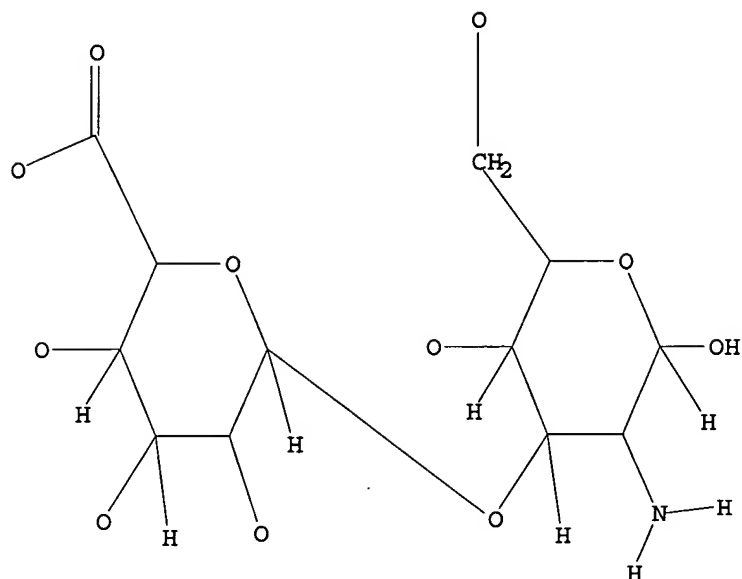


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=> d L1
L1 HAS NO ANSWERS
L1 STR
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Structure attributes must be viewed using STN Express query preparation.

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=> s L1 sss sam
SAMPLE SEARCH INITIATED 16:51:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1196 TO ITERATE

100.0% PROCESSED 1196 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                        BATCH **COMPLETE**
PROJECTED ITERATIONS: 21846 TO 25994
PROJECTED ANSWERS: 0 TO 0
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L2 0 SEA SSS SAM L1
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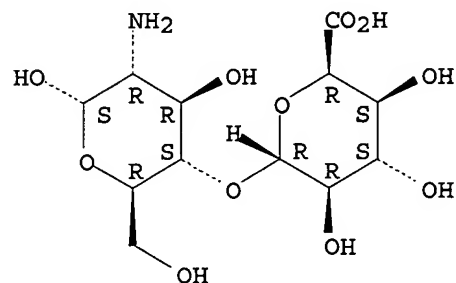
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=> s L1 sss full
FULL SEARCH INITIATED 16:51:37 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 23877 TO ITERATE
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100.0% PROCESSED 23877 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01
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L3 4 SEA SSS FUL L1
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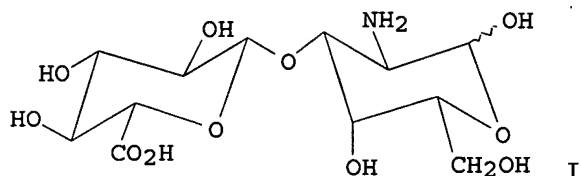
L6 13 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN  
IN  $\alpha$ -D-Glucopyranose, 2-amino-2-deoxy-4-O- $\alpha$ -L-idopyranuronosyl-  
(9CI)  
MF C12 H21 N O11

Absolute stereochemistry.



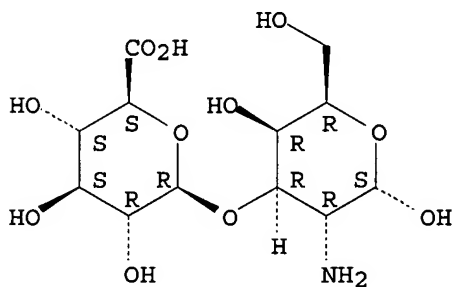
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L7 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1992:571900 CAPLUS  
 DOCUMENT NUMBER: 117:171900  
 TITLE: Evidence for a boat-chair equilibrium in the  
 glucuronate residue of chondrosine  
 AUTHOR(S): Lamba, Dorian; Segre, Anna Laura; Ragazzi, Massimo;  
 Ferro, Dino Romano; Toffanin, Renato  
 CORPORATE SOURCE: Ist. Strutt. Chim. "Giordano Giacomello", CNR,  
 Monterotondo Stazione Rome, I-00016, Italy  
 SOURCE: Carbohydrate Research (1991), 209, C13-C15  
 CODEN: CRBRAT; ISSN: 0008-6215  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



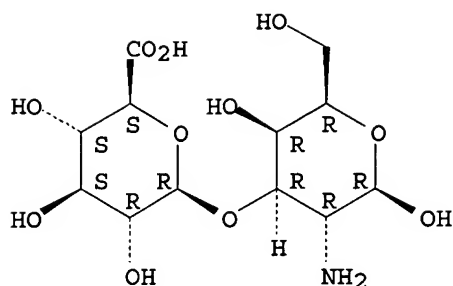
AB The first exptl. and computational evidence for a boat-like conformation  
 of the glucuronate ring in chondrosine (I), is reported.  
 IT 140866-46-2 143521-24-8  
 RL: PRP (Properties)  
 (conformation of, NMR in relation to)  
 RN 140866-46-2 CAPLUS  
 CN  $\alpha$ -D-Galactopyranose, 2-amino-2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



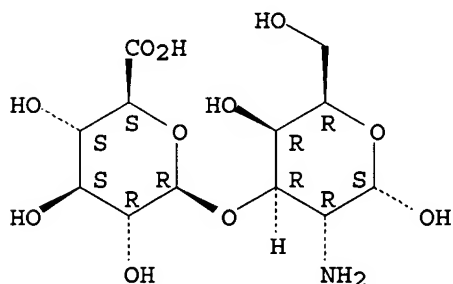
RN 143521-24-8 CAPLUS  
 CN  $\beta$ -D-Galactopyranose, 2-amino-2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-  
 (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1992:214810 CAPLUS  
 DOCUMENT NUMBER: 116:214810  
 TITLE: Analysis of glycosaminoglycan-derived oligosaccharides using fast-atom-bombardment mass spectrometry  
 AUTHOR(S): Linhardt, Robert J.; Wang, Hui M.; Loganathan, Duraikkannu; Lamb, Diane J.; Mallis, Larry M.  
 CORPORATE SOURCE: Coll. Pharm., Univ. Iowa, Iowa City, IA, 52242, USA  
 SOURCE: Carbohydrate Research (1992), 225(1), 137-45  
 CODEN: CRBRAT; ISSN: 0008-6215  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB A method of performing fast-atom-bombardment mass spectrometry (f.a.b. ms) anal. on glycosaminoglycan-derived oligosaccharides obtained from heparin using triethanolamine, as the liquid f.a.b. matrix, in the neg.-ion mode, is reported.  
 IT 140866-46-2P  
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and fast-atom-bombardment mass spectra of)  
 RN 140866-46-2 CAPLUS  
 CN  $\alpha$ -D-Galactopyranose, 2-amino-2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1988:56539 CAPLUS  
 DOCUMENT NUMBER: 108:56539  
 TITLE: Preparation of oligosaccharides consisting of a uronic acid and a hexosamine as hair growth promoters  
 INVENTOR(S): Couchman, John Robert; Gibson, Walter Thomas  
 PATENT ASSIGNEE(S): Unilever PLC, UK; Unilever N. V.  
 SOURCE: Eur. Pat. Appl., 107 pp.  
 CODEN: EPXXDW  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 211610	A2	19870225	EP 1986-305853	19860730
EP 211610	A3	19880224		
EP 211610	B1	19930915		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
CA 1334656	A1	19950307	CA 1986-514616	19860724
US 4761401	A	19880802	US 1986-891940	19860729
AU 8660717	A1	19870205	AU 1986-60717	19860730
AU 570366	B2	19880310		
BR 8603606	A	19870310	BR 1986-3606	19860730
IN 165624	A	19891125	IN 1986-BO214	19860730
EP 354595	A1	19900214	EP 1989-117874	19860730
EP 354595	B1	19930224		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 85884	E	19930315	AT 1989-117874	19860730
AT 94554	E	19931015	AT 1986-305853	19860730
JP 62036394	A2	19870217	JP 1986-181204	19860731
ZA 8605732	A	19880427	ZA 1986-5732	19860731
JP 03072412	A2	19910327	JP 1990-194687	19900723
JP 07103009	B4	19951108		

PRIORITY APPLN. INFO.:

GB 1985-19416	A	19850801
EP 1986-305853	P	19860730
EP 1989-117874	A	19860730

OTHER SOURCE(S): MARPAT 108:56539

GI For diagram(s), see printed CA Issue.

AB Esterified oligosaccharides (I), consisting of uronic acids II [R1 = C3-10 alkyl, CH(CO2R2)(CH2)nMe; n = 0-7; R2 = H, C1-4 alkyl, CO(CH2)mMe, SO3M; m = 0-2; M = H, metal or organic cation] and hexosamines III [R3 = H, CO(CH2)mMe, SO3M], provided that R2 is the same or different and 1 R2 has a pyranose ring structure linked by  $\alpha$ -1,3,  $\alpha$ -1,4,  $\beta$ -1,3, or  $\beta$ -1,4 glycosidic linkage, and disaccharides IV and V, were prepared as a hair growth promoters, useful in baldness cures (no data). Chondrosin, obtained by acid hydrolysis of chondroitin sulfate in 2N H2SO4, was selectively N-acetylated, sulfated at the 6-position by Et3NSO3H, esterified with Me(CH2)5OH, and peracetylated to give V [R1 = Me(CH2)5, R2 = Ac].

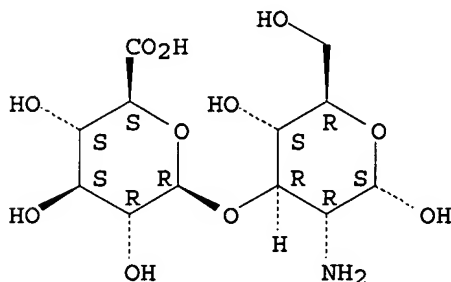
IT 112464-83-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as hair growth promoter)

RN 112464-83-2 CAPLUS

CN  $\alpha$ -D-Glucopyranose, 2-amino-2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-  
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L7 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1975:50114 CAPLUS

DOCUMENT NUMBER: 82:50114

TITLE: Structural study of mucopolysaccharides. Crystal

structure of chondrosine monohydrate  
 AUTHOR(S): Senma, Masanori; Taga, Tooru; Osaki, Kenji  
 CORPORATE SOURCE: Fac. Pharm. Sci., Kyoto Univ., Kyoto, Japan  
 SOURCE: Chemistry Letters (1974), (12), 1415-18  
 CODEN: CMLTAG; ISSN: 0366-7022  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB The structure of chondrosine monohydrate was determined by an x-ray study. The zwitterionic character of the mol. and the intermol. H bonds stabilize the crystal structure. An intramol. H bond is found between the axial oxygen O(4') and the ring oxygen O(5). The galactosamine moiety has an  $\alpha$ -configuration in the crystalline state.

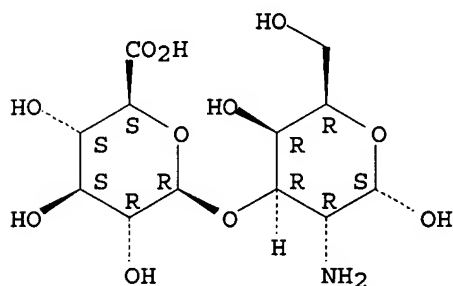
IT 54575-84-7

RL: PRP (Properties)  
 (crystal structure of)

RN 54575-84-7 CAPLUS

CN  $\alpha$ -D-Galactopyranose, 2-amino-2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-, monohydrate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● H<sub>2</sub>O

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:205384 CAPLUS

DOCUMENT NUMBER: 140:319839

TITLE: A structural and dynamic model for the interaction of interleukin-8 and glycosaminoglycans: support from isothermal fluorescence titrations

AUTHOR(S): Krieger, Elmar; Geretti, Elena; Brandner, Barbara; Goger, Birgit; Wells, Timothy N.; Kungl, Andreas J.

CORPORATE SOURCE: Centre for Molecular and Biomolecular Informatics, Nijmegen, Neth.

SOURCE: Proteins: Structure, Function, and Bioinformatics (2004), 54(4), 768-775

CODEN: PSFBAF

PUBLISHER: Wiley-Liss, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Binding of interleukin-8 (IL-8) to glycosaminoglycans (GAGs) on the surface of endothelial cells is crucial for the recruitment of neutrophils to an inflammatory site. Deriving structural knowledge about this interaction from in silico docking expts. has proved difficult because of the high flexibility and the size of GAGs. Therefore, the authors developed a docking method that takes into account ligand and protein flexibility by running .apprx.15,000 mol. dynamics simulations of the docking event with different initial orientations of the binding partners. The method was shown to successfully reproduce the residues of basic fibroblast growth factor involved in GAG binding. Docking of a heparin hexasaccharide to IL-8 gave an interaction interface involving the basic residues His18, Lys20, Arg60, Lys64, Lys67, and Arg68. By subjecting IL-8 single-site mutants, in which these amino acids were replaced by alanine, to isothermal fluorescence titrns., the affinities for heparin were determined to be wtIL-8 > IL-8(H18A) » IL-8(R68A) > IL-8(K67A) » IL-8(K20A) > IL-8(R60A) » IL-8(K64A). A comparison with the binding energies calculated from the model revealed high values for wtIL-8 and the H18A mutant and significantly lower but similar energies for the remaining mutants. Connecting the two fully sulfated hexasaccharides bound to each of the two IL-8 monomers in the dimeric chemokine by an N-acetylated dodecasaccharide gave a complex structure in which the GAG mol. aligned in a parallel fashion to the N-terminal  $\alpha$ -helixes of IL-8 like a horseshoe. A 5-ns mol. dynamics simulation of this complex confirmed its structural stability and revealed a reorientation in both binding sites where a disaccharide became the central binding unit. Isothermal fluorescence titration expts. using differently sulfated heparin disaccharides confirmed that a single disaccharide can indeed bind IL-8 with high affinity.

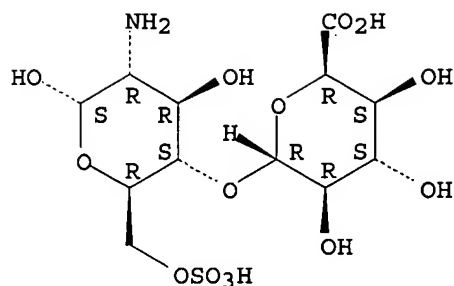
IT 140946-24-3 677750-87-7

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)  
(of heparin in binding to interleukin-8)

RN 140946-24-3 CAPLUS

CN  $\alpha$ -D-Glucopyranose, 2-amino-2-deoxy-4-O- $\alpha$ -L-idopyranuronosyl-, 6-(hydrogen sulfate) (9CI) (CA INDEX NAME)

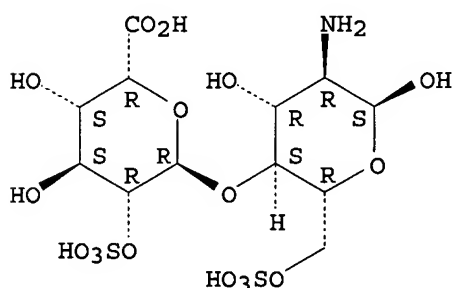
Absolute stereochemistry.



RN 677750-87-7 CAPLUS

CN α-D-Glucopyranose, 2-amino-2-deoxy-4-O-(2-O-sulfo-α-L-idopyranuronosyl)-, 6-(hydrogen sulfate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:151894 CAPLUS

DOCUMENT NUMBER: 132:274439

TITLE: An NMR and Molecular Modeling Study of the Site-Specific Binding of Histamine by Heparin, Chemically Modified Heparin, and Heparin-Derived Oligosaccharides

AUTHOR(S): Chuang, Wei-Lien; Christ, Marie Dvorak; Peng, Jie; Rabenstein, Dallas L.

CORPORATE SOURCE: Department of Chemistry, University of California Riverside, Riverside, CA, 92521, USA

SOURCE: Biochemistry (2000), 39(13), 3542-3555  
CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The diprotonated form of histamine binds site-specifically to heparin, a highly sulfated 1→4 linked repeating copolymer comprised predominantly of 2-O-sulfo-α-L-iduronic acid (the I ring) and 2-deoxy-2-sulfamido-6-O-sulfo-α-D-glucopyranosyl (the A ring). The binding is mediated by electrostatic interactions. The structural features of histamine and heparin, which are required for the site-specific binding, have been identified from the results of <sup>1</sup>H NMR studies of the binding of histamine by six heparin-derived oligosaccharides and four chemical modified heparins and mol. modeling studies. The results indicate that the imidazolium ring of diprotonated histamine is critical for directing site-specific binding, while the ammonium group increases the binding affinity. The imidazolium ring binds within a cleft, with the A ring of an IAI triad at the top of the cleft, and the I rings forming the two sides. The H3 proton of the A ring is in the shielding cone of the imidazolium ring. The carboxylate group of the



I-ring at the reducing end of the IAI triad and possibly the sulfamido group of the A-ring are essential for site-specific binding, whereas the 2-O-sulfate group of the I ring and the 6-O-sulfate group of the A ring are not. The results indicate that histamine binds to the IAI triad with the I rings in the <sup>1</sup>C<sub>4</sub> conformation. Also, the configuration of the carboxylate group is critical, as indicated by the absence of site-specific binding of histamine by the related IAG sequence, where G is α-D-glucuronic acid. The mol. modeling results indicate that the N1H and N3H protons of the imidazolium ring of site-specifically bound histamine are hydrogen bonded to the carboxylates of the I rings at the nonreducing and reducing ends of the IAI trisaccharide sequence.

IT 263904-72-9

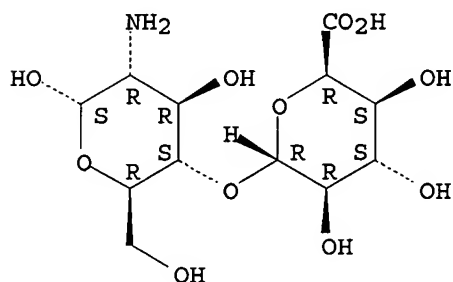
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(repeating unit of; NMR and mol. modeling of site-specific binding of histamine by heparin and chemical modified heparin and heparin-derived oligosaccharides)

RN 263904-72-9 CAPLUS

CN α-D-Glucopyranose, 2-amino-2-deoxy-4-O-α-L-idopyranuronosyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:140917 CAPLUS

DOCUMENT NUMBER: 123:33555

TITLE: Heparin-like compounds prepared by chemical modification of capsular polysaccharide from E. coli K5

AUTHOR(S): Casu, Benito; Grazioli, Giordana; Razi, Nahid; Guerrini, Marco; Naggi, Annamaria; Torri, Giangiacomo; Oreste, Pasqua; Tursi, Francesco; Zoppetti, Giorgio; et al.

CORPORATE SOURCE: Istituto di Chimica e Biochimica G. Ronzoni, Milan, Italy

SOURCE: Carbohydrate Research (1994), 263(2), 271-84  
CODEN: CRBRAT; ISSN: 0008-6215

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

→ 4-?-D-GlcA(1→4)-?-D-GlcNSO<sub>3</sub><sup>-</sup>-(1→ I

AB O-Sulfation of sulfaminoheparosan SAH, a glycosaminoglucuronan I, obtained

by N-deacetylation and N-sulfation of the capsular polysaccharide from *E. coli* K5, was investigated in order to characterize the sulfation pattern eliciting heparin-like activities. SAH was reacted (as the tributylammonium salt in *N,N*-dimethylformamide) with pyridine-sulfur trioxide under systematically different exptl. conditions. The structure of O-sulfated products (SAHS), as determined by mono- and two-dimensional <sup>1</sup>H and <sup>13</sup>C NMR, varied with variation of reaction parameters. Sulfation of SAH preferentially occurred at O-6 of the GlcNSO-3 residues. Further sulfation occurred either at O-3 or at O-2 of the GlcA residues, depending on the exptl. conditions. Products with significantly high affinity for antithrombin and anti-factor Xa activity were obtained under well-defined conditions. These products contained the trisulfated amino sugar GlcNSO-3,3,6SO-3, which is a marker component of the pentasaccharide sequence through which heparin binds to antithrombin.

IT 164082-45-5P

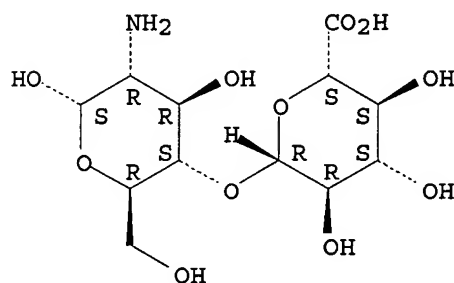
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(heparin-like compds. prepared by chemical modification of capsular polysaccharide from *E. coli*)

RN 164082-45-5 CAPLUS

CN α-D-Glucopyranose, 2-amino-2-deoxy-4-O-β-D-glucopyranuronosyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1992:210107 CAPLUS

DOCUMENT NUMBER: 116:210107

TITLE: Human α-L-iduronidase. Catalytic properties and an integrated role in the lysosomal degradation of heparan sulfate

AUTHOR(S): Freeman, Craig; Hopwood, John J.

CORPORATE SOURCE: Dep. Chem. Pathol., Adelaide Child. Hosp., North Adelaide, 5006, Australia

SOURCE: Biochemical Journal (1992), 282(3), 899-908  
CODEN: BIJOAK; ISSN: 0306-3275

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The kinetic parameters (*K<sub>m</sub>* and *k<sub>cat</sub>*.) of human liver α-L-iduronidase were determined with a variety of heparin-derived disaccharide and tetrasaccharide substrates. More structural complex substrates, in which several aspects of the aglycon structure of the natural substrates heparin and heparan sulfate were maintained, were hydrolyzed with catalytic efficiencies up to 255-times that observed for the simplest disaccharide substrate to be hydrolyzed. The major aglycon structure that influenced both substrate binding and enzyme activity was the presence of a C-6 sulfate ester on the residue adjacent to the iduronic acid residue being hydrolyzed. Sulfate ions and a number of substrate and product analogs were potent inhibitors of enzyme activity. Human liver α-L-iduronidase activity towards 4-methylumbelliferyl α-L-iduronide at pH 4.8 had two *K<sub>m</sub>* values of 37 μM and 1.92 mM with corresponding *k<sub>cat</sub>* values of

299 and 650 mol of product formed/min per mol of enzyme resp., which may explain the wide range of  $K_m$  values previously reported for  $\alpha$ -L-iduronidase activity toward its substrate. Skin fibroblast  $\alpha$ -L-iduronidase activity towards the heparin-derived oligosaccharides was influenced by the same substrate aglycon structural features as was observed for the human liver enzyme. A comparison was made of the effect of substrate aglycon structure upon catalytic activities of the enzymes which act to degrade the highly sulfated regions of heparan sulfate. A model was proposed whereby the substrate is directed from  $\alpha$ -L-iduronidase to subsequent enzyme activities to ensure the efficient degradation of heparan sulfate.

IT 141043-27-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with iduronidase of human, structure in relation to)

RN 141043-27-8 CAPLUS

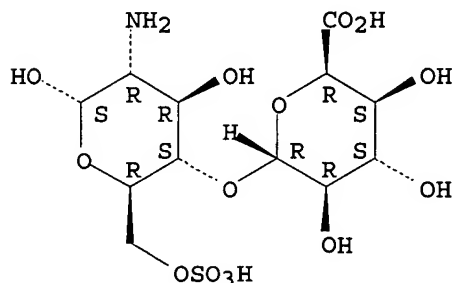
CN D-Mannitol, O- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ ?) -O-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 3)-2,5-anhydro-, 1-(hydrogen sulfate) (9CI)  
(CA INDEX NAME)

CM 1

CRN 140946-24-3

CMF C12 H21 N O14 S

Absolute stereochemistry.

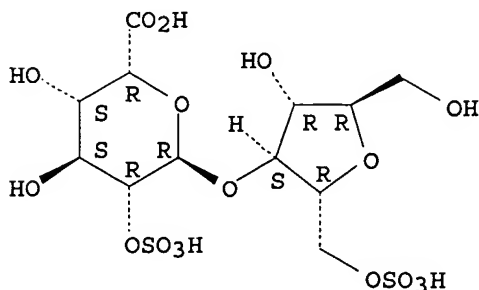


CM 2

CRN 69180-27-4

CMF C12 H20 O17 S2

Absolute stereochemistry.



L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:7066 CAPLUS

DOCUMENT NUMBER: 100:7066

TITLE: Organic oligosaccharides, corresponding to fragments

of natural mucopolysaccharides, and their biological applications

INVENTOR(S) :

Petitou, Maurice; Jacquinet, Jean Claude; Sinay, Pierre; Choay, Jean; Lormeau, Jean Claude; Nassr, Mahmoud

PATENT ASSIGNEE(S) :

Choay S. A., Fr.

SOURCE :

Eur. Pat. Appl., 187 pp.

CODEN: EPXXDW

DOCUMENT TYPE :

Patent

LANGUAGE :

French

FAMILY ACC. NUM. COUNT :

5

PATENT INFORMATION :

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 84999	A1	19830803	EP 1983-400110	19830117
EP 84999	B1	19880413		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
FR 2519987	A1	19830722	FR 1982-621	19820115
FR 2520744	A1	19830805	FR 1982-1575	19820201
FR 2521566	A1	19830819	FR 1982-2526	19820216
FR 2527614	A1	19831202	FR 1982-9392	19820528
FR 2528853	A1	19831223	FR 1982-10891	19820622
FR 2528854	A1	19831223	FR 1982-10892	19820622
FR 2529557	A1	19840106	FR 1982-11679	19820702
FR 2531436	A1	19840210	FR 1982-13804	19820806
FR 2533219	A1	19840323	FR 1982-15803	19820920
FR 2533220	A1	19840323	FR 1982-15804	19820920
FR 2535324	A1	19840504	FR 1982-18003	19821027
US 4987223	A	19910122	US 1982-453731	19821027
CA 1265132	A1	19900130	CA 1983-419417	19830113
DK 8300143	A	19830716	DK 1983-143	19830114
DK 174348	B1	20021223		
AU 8310397	A1	19830721	AU 1983-10397	19830114
AU 563351	B2	19870709		
JP 58170797	A2	19831007	JP 1983-5178	19830114
JP 05065517	B4	19930917		
ES 519232	A1	19840316	ES 1983-519232	19830114
SU 1694065	A3	19911123	SU 1983-3545151	19830114
AT 33496	E	19880415	AT 1983-400110	19830117
AU 8321285	A1	19840522	AU 1983-21285	19831027
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DK 8403135	A	19840627	DK 1984-3135	19840627
DK 175970	B1	20051003		
US 4943630	A	19900724	US 1986-856855	19860421
JP 05331182	A2	19931214	JP 1992-115407	19920408
JP 2510454	B2	19960626		

PRIORITY APPLN. INFO.:

FR 1982-621	A	19820115
FR 1982-1575	A	19820201
FR 1982-2526	A	19820216
FR 1982-9392	A	19820528
FR 1982-10891	A	19820622
FR 1982-10892	A	19820622
FR 1982-11679	A	19820702
FR 1982-13804	A	19820806
FR 1982-15803	A	19820920
FR 1982-15804	A	19820920
FR 1982-18003	A	19821027
FR 1981-24132	A	19811223
FR 1982-18001	A	19821027
EP 1983-400110	A	19830117

EP 1983-402109

A 19831027

WO 1983-FR217

A 19831027

US 1984-624628

A 19840626

OTHER SOURCE(S): CASREACT 100:7066

GI For diagram(s), see printed CA Issue.

AB Mucopolysaccharide fragments were synthesized. Thus the pentasaccharide I was prepd from the monosaccharides in a synthesis comprising many steps. I has factor Xa antagonist activity >2000 U/mg.

IT 87907-17-3P 87907-41-3P 87907-42-4P

87907-52-6P

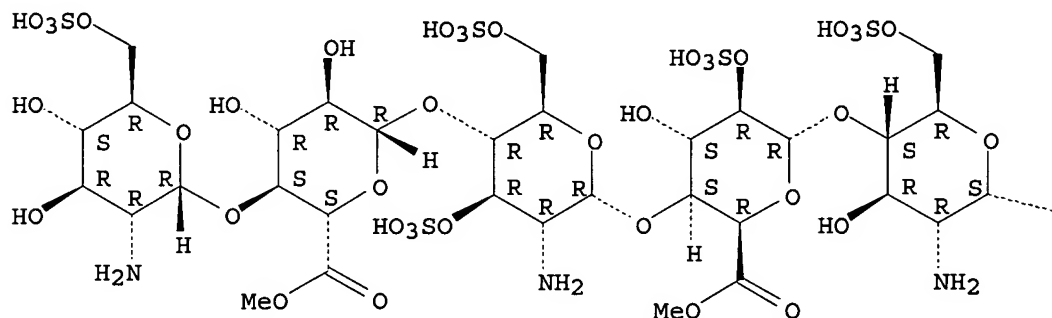
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and sulfonylation of)

RN 87907-17-3 CAPLUS

CN  $\alpha$ -D-Glucopyranose, O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-methyl- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-methyl-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate), pentasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● 5 Na

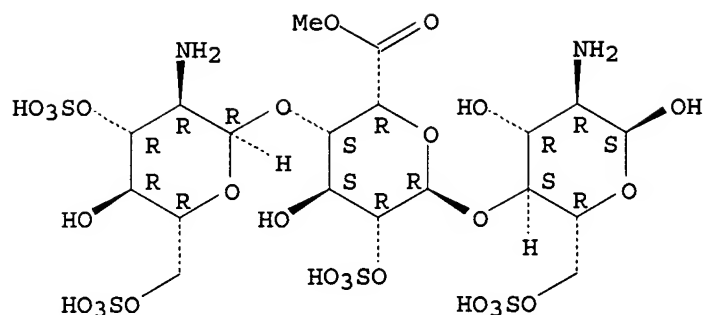
PAGE 1-B

OH

RN 87907-41-3 CAPLUS

CN  $\alpha$ -D-Glucopyranose, O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-methyl-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate) (9CI)  
(CA INDEX NAME)

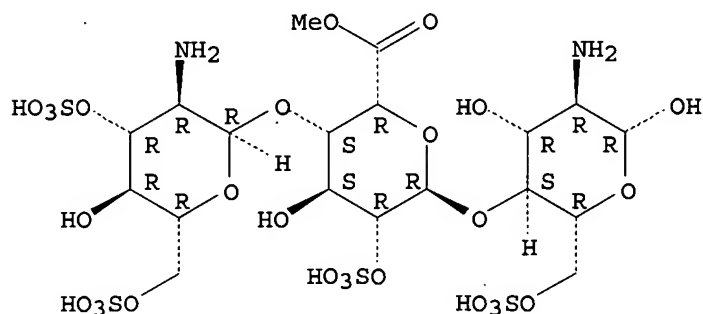
Absolute stereochemistry.



RN 87907-42-4 CAPLUS

CN  $\beta$ -D-Glucopyranose, O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-methyl-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate) (9CI)  
(CA INDEX NAME)

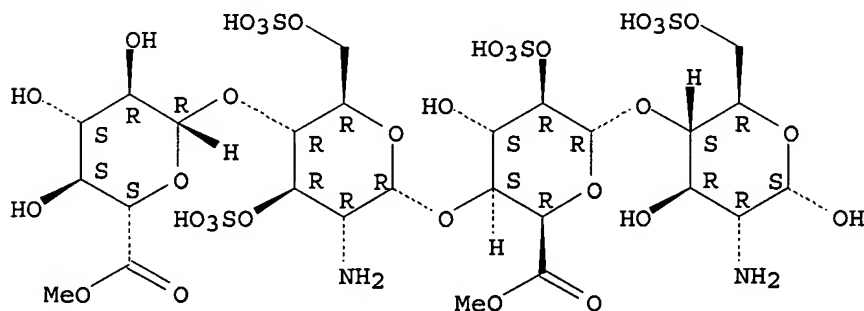
Absolute stereochemistry.



RN 87907-52-6 CAPLUS

CN  $\alpha$ -D-Glucopyranose, O-6-methyl- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-methyl-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-2-amino-2-deoxy-, 6-(hydrogen sulfate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 87925-82-4P 87925-84-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

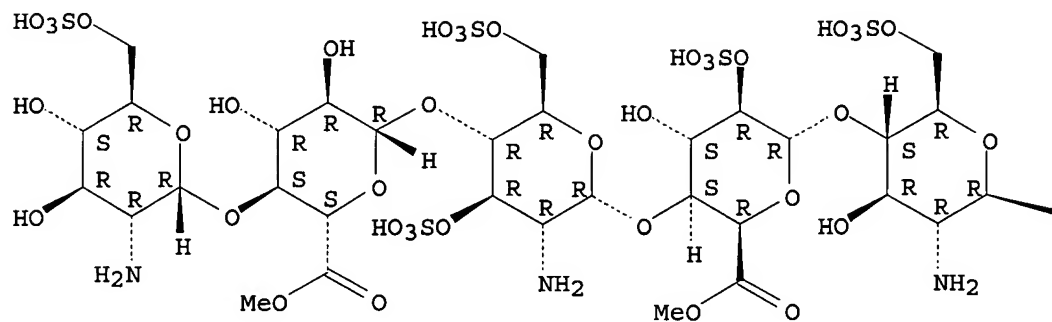
RN 87925-82-4 CAPLUS

CN  $\beta$ -D-Glucopyranose, O-2-amino-2-deoxy-6-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-methyl- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 4)-O-2-amino-2-deoxy-3,6-di-O-sulfo- $\alpha$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-methyl-2-O-sulfo- $\alpha$ -L-idopyranuronosyl-(1 $\rightarrow$ 4)-

2-amino-2-deoxy-, 6-(hydrogen sulfate), pentasodium salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



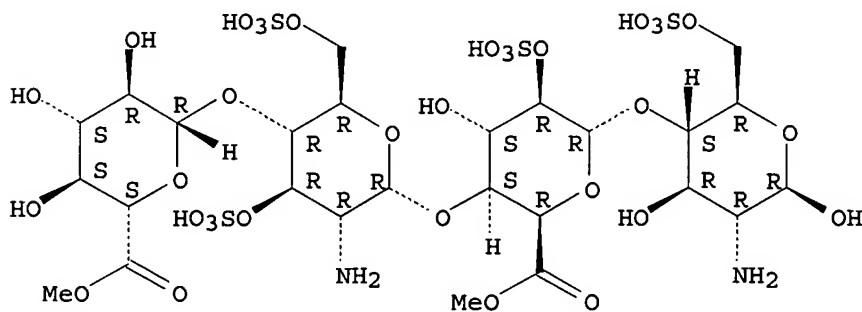
● 5 Na

PAGE 1-B

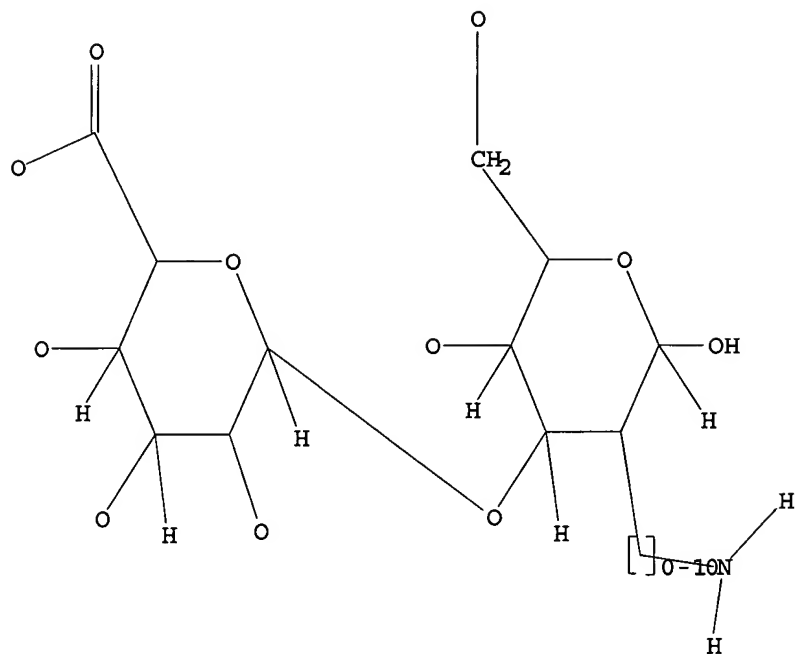
OH

RN 87925-84-6 CAPLUS  
 CN β-D-Glucopyranose, O-6-methyl-β-D-glucopyranuronosyl-(1→4)-O-2-amino-2-deoxy-3,6-di-O-sulfo-α-D-glucopyranosyl-(1→4)-O-6-methyl-2-O-sulfo-α-L-idopyranuronosyl-(1→4)-2-amino-2-deoxy-, 6-(hydrogen sulfate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



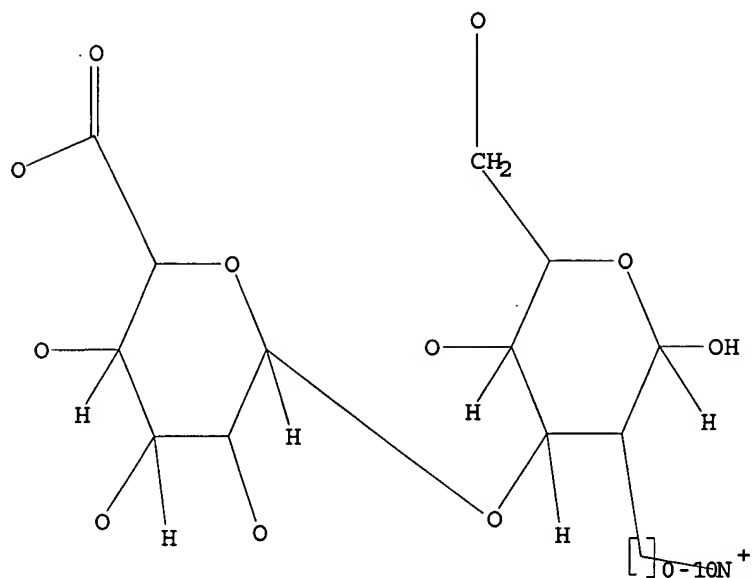
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L9 HAS NO ANSWERS  
L9 STR



Structure attributes must be viewed using STN Express query preparation.

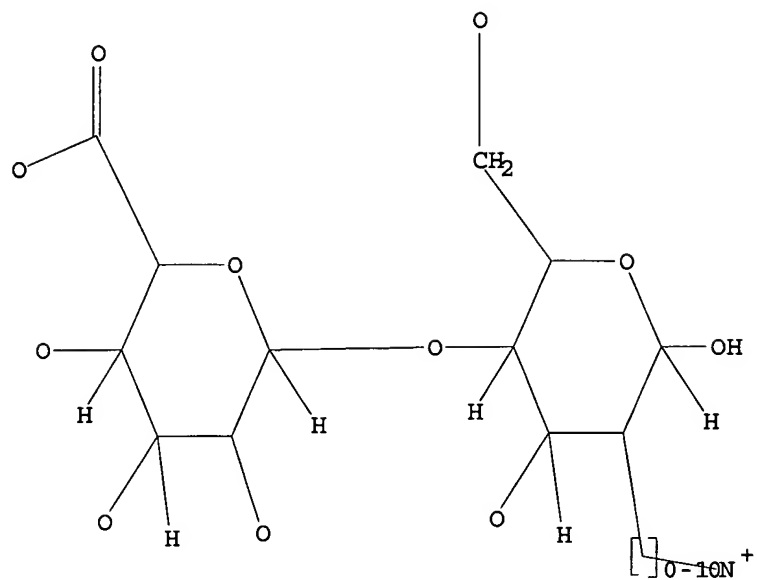


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 L15 STR



Structure attributes must be viewed using STN Express query preparation.

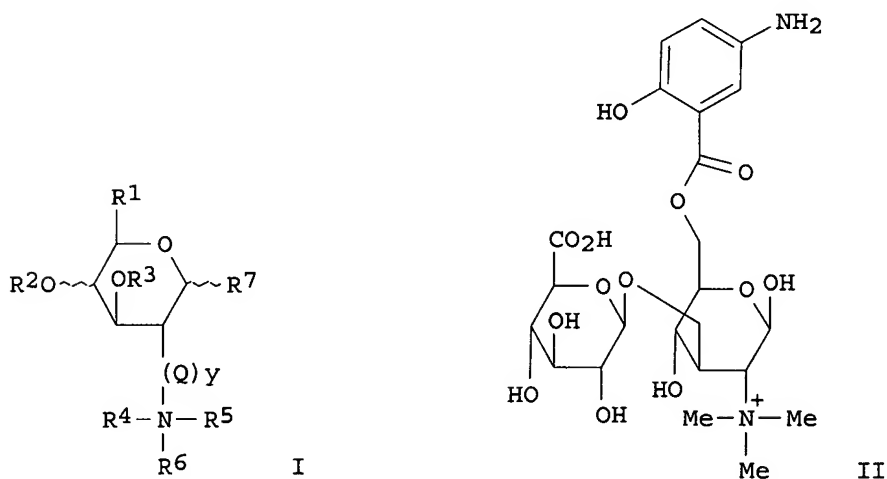
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 L18 STR



Structure attributes must be viewed using STN Express query preparation.

ACCESSION NUMBER: 2004:589230 CAPLUS  
 DOCUMENT NUMBER: 141:123864  
 TITLE: Preparation of aminodeoxy oligosaccharide as anti-inflammatory agents and their bio-adhesive pharmaceutical compositions  
 INVENTOR(S): Barbeau, Donald L.  
 PATENT ASSIGNEE(S): USA  
 SOURCE: U.S. Pat. Appl. Publ., 42 pp., Cont.-in-part of U.S. Ser. No. 348,851.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004142880	A1	20040722	US 2004-760970	20040120
US 6699848	B1	20040302	US 2003-348851	20030122
CA 2513304	AA	20040805	CA 2004-2513304	20040121
PRIORITY APPLN. INFO.:			US 2003-348851	A2 20030122
			US 2004-760970	A 20040120
			WO 2004-US1536	W 20040121
OTHER SOURCE(S):		MARPAT 141:123864		
GI				



AB Aminodeoxy sugars I, wherein Q is a lower alkylene, R<sup>1</sup> is CH<sub>2</sub>-O-(linker)n-R, CO-O-(linker)n-R, CO-NH-(linker)n-R; n is 0, 1; yr is 0, 1; R is H, pharmacol. active drug residue; R<sup>2</sup> is H, monosaccharide residue, oligosaccharide residue; R<sup>3</sup> is H, monosaccharide residue, oligosaccharide residue, CH(CH<sub>2</sub>)C(O)OCH<sub>2</sub>OR<sub>8</sub>; a monomeric glycoside or an oligomeric glycoside; R<sup>4</sup>-R<sup>6</sup> are independently hydrogen, alkyl, aryl, aralkyl, and cycloalkyl or together form a nitrogen-containing ring, and R<sup>7</sup> is hydroxyl or hydroxyalkyl; R<sub>8</sub> a pharmacol. active drug residue. The chronic inflammation in Crohn's disease involves any level of the gastrointestinal tract, and leads to progressive damage in the mucosa, submucosa, the deeper longitudinal muscle layers serosa and regional lymph nodes. Crohn's disease involvement of the mucosa includes confluent linear ulceration patchy, and sharply demarcated granulomas. Thus,

disaccharide uronate II was prepared and tested as anti-inflammatory agent. The invention further relates to a method of controlling the delivery of anti-inflammatory compds., particularly mesalamine (5-amino salicylic acid, 5-ASA), 4-amino salicylic acid (4-ASA), and 3-amino salicylic acid (3-ASA) to the entire gastrointestinal (GI) tract in patients suffering from inflammatory bowel disease. The compns. of the present invention can target a site throughout the length of the gastrointestinal intestinal tract to consistently deliver the medicine where it will be clin. most effective. The compds. of the present invention are characterized by low octanol:water coeffs. and mol. wts. greater than about 300 g/mol. The prodrugs of the present invention are further characterized by their functional properties, including but not limited to bio-adhesion and controlled hydrolysis of the active anti-inflammatory compds.

IT 664342-94-3P 722500-26-7P

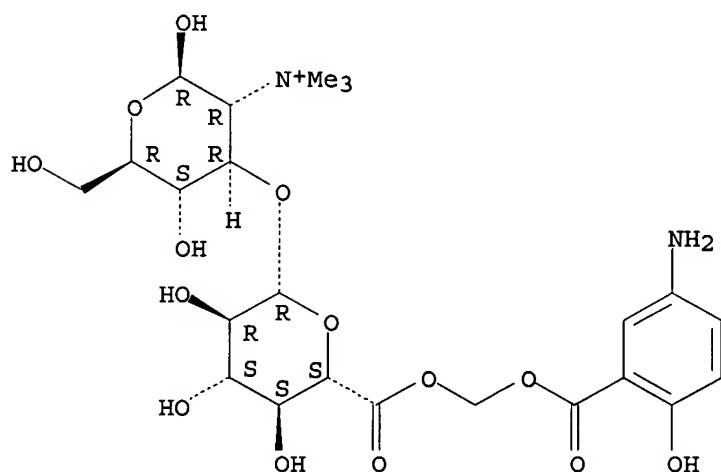
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of aminodeoxy oligosaccharide as anti-inflammatory agents and their bio-adhesive pharmaceutical compns.)

RN 664342-94-3 CAPLUS

CN  $\beta$ -D-Glucopyranose, 3-O-[6-[[[(5-amino-2-hydroxybenzoyl)oxy]methyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)-(9CI) (CA INDEX NAME)

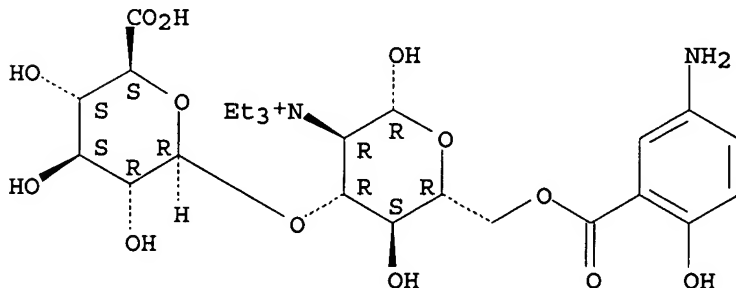
Absolute stereochemistry.



RN 722500-26-7 CAPLUS

CN  $\beta$ -D-Glucopyranose, 2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-2-(triethylammonio)-, 6-(5-amino-2-hydroxybenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 664342-93-2P 722500-10-9P 722500-27-8P  
 722500-28-9P 722500-29-0P 722500-30-3P  
 722500-31-4P 722500-32-5P 722500-33-6P  
 722500-36-9P 722500-39-2P

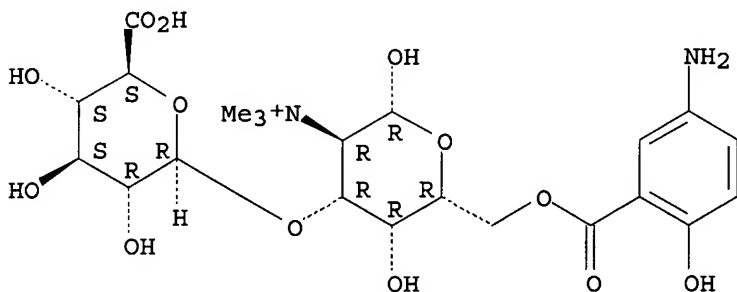
RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminodeoxy oligosaccharide as anti-inflammatory agents and their bio-adhesive pharmaceutical compns.)

RN 664342-93-2 CAPLUS

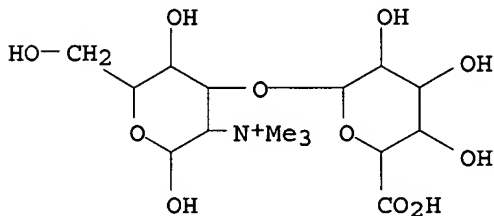
CN  $\beta$ -D-Galactopyranose, 2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-2-(trimethylammonio)-, 6-(5-amino-2-hydroxybenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 722500-10-9 CAPLUS

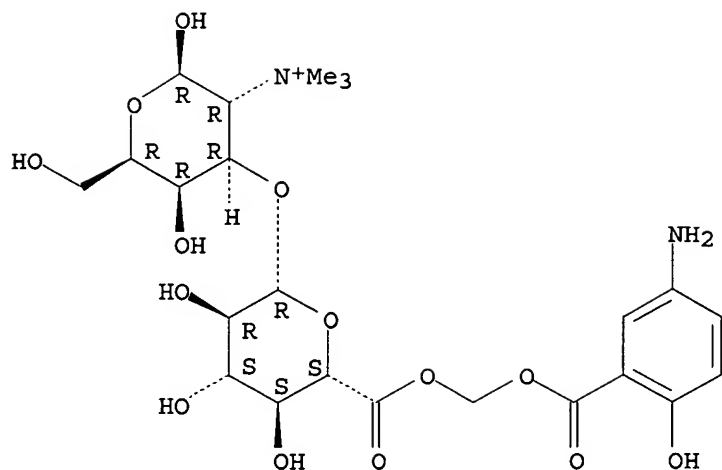
CN Hexopyranose, 2-deoxy-3-O-hexopyranuronosyl-2-(trimethylammonio)- (9CI) (CA INDEX NAME)



RN 722500-27-8 CAPLUS

CN  $\beta$ -D-Galactopyranose, 3-O-[6-[[5-amino-2-hydroxybenzoyl]oxy]methyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

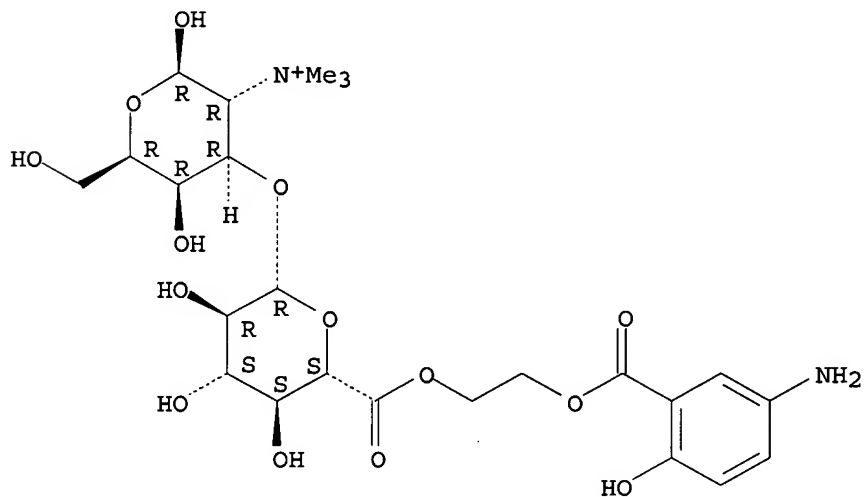
Absolute stereochemistry.



RN 722500-28-9 CAPLUS

CN  $\beta$ -D-Galactopyranose, 3-O-[6-[2-[(5-amino-2-hydroxybenzoyl)oxy]ethyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

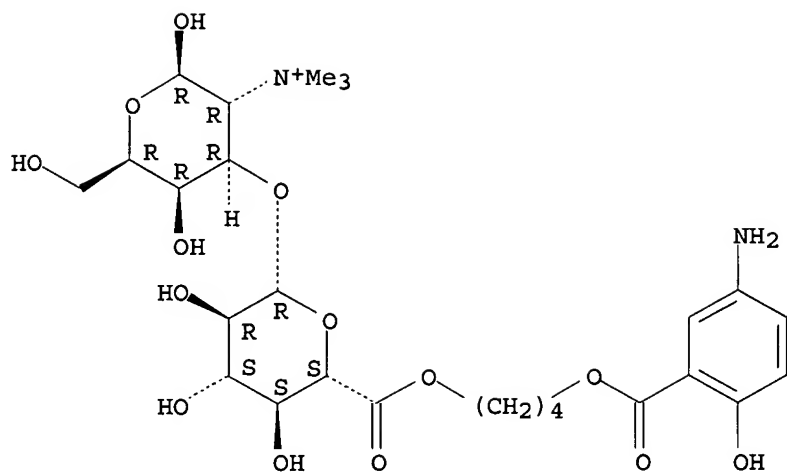
Absolute stereochemistry.



RN 722500-29-0 CAPLUS

CN  $\beta$ -D-Galactopyranose, 3-O-[6-[4-[(5-amino-2-hydroxybenzoyl)oxy]butyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

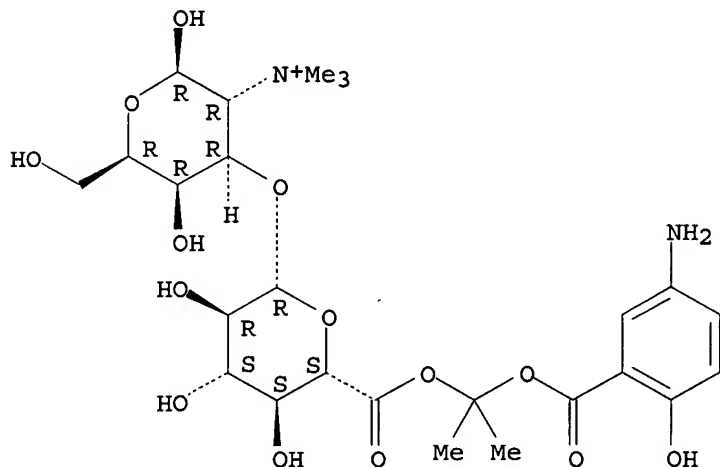
Absolute stereochemistry.



RN 722500-30-3 CAPLUS

CN  $\beta$ -D-Galactopyranose, 3-O-[6-[1-[(5-amino-2-hydroxybenzoyl)oxy]-1-methylethyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)-(9CI) (CA INDEX NAME)

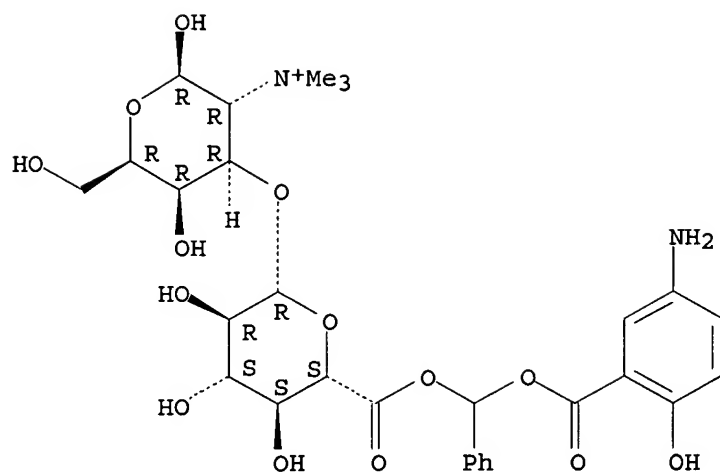
Absolute stereochemistry.



RN 722500-31-4 CAPLUS

CN  $\beta$ -D-Galactopyranose, 3-O-[6-[[[5-amino-2-hydroxybenzoyl)oxy]phenylmethyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

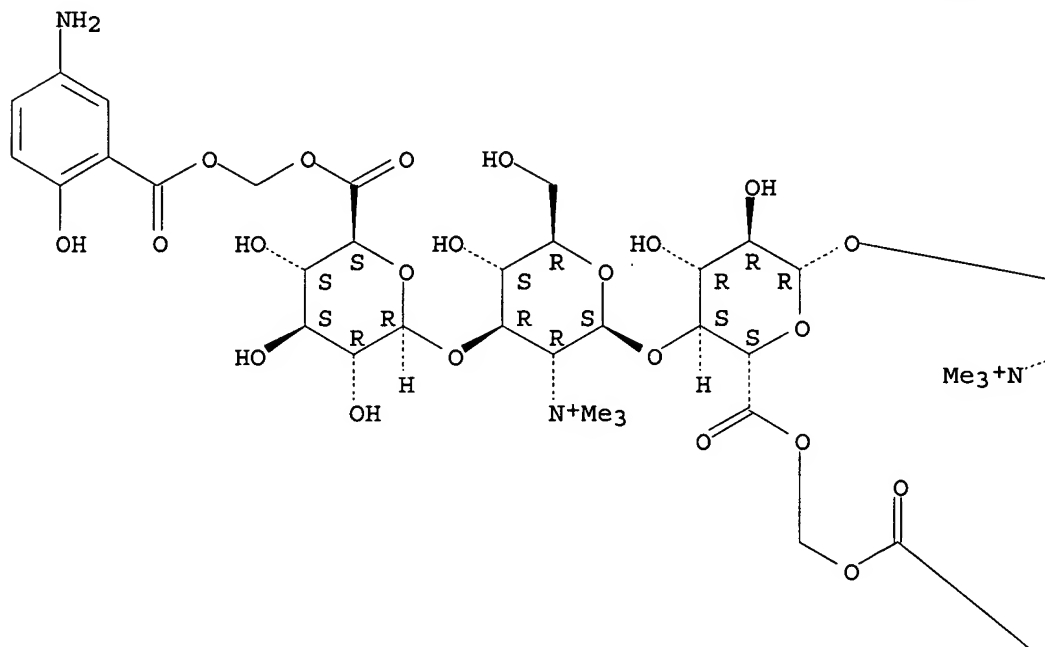


RN 722500-32-5 CAPLUS

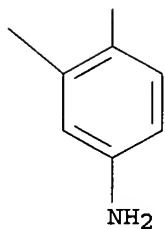
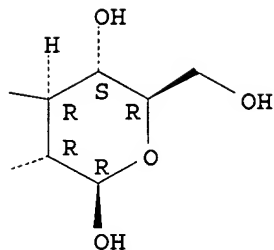
CN  $\beta$ -D-Glucopyranose, O-6-[[ (5-amino-2-hydroxybenzoyl)oxy]methyl]- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 3)-O-2-deoxy-2-(trimethylammonio)- $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O-6-[[ (5-amino-2-hydroxybenzoyl)oxy]methyl]- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 3)-2-deoxy-2-(trimethylammonio)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

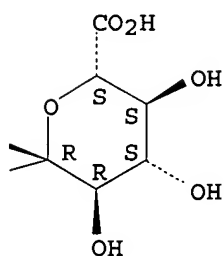
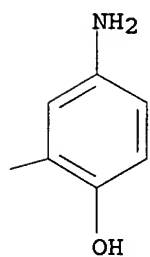
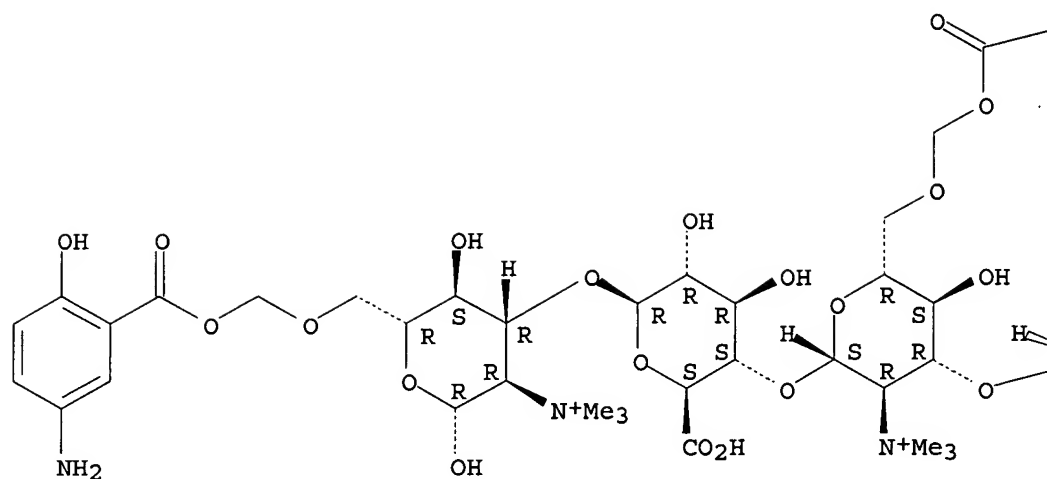






RN 722500-33-6 CAPLUS  
 CN  $\beta$ -D-Glucopyranose, O- $\beta$ -D-glucopyranuronosyl-(1 $\rightarrow$ 3)-O-6-O-  
 [[(5-amino-2-hydroxybenzoyl)oxy]methyl]-2-deoxy-2-(trimethylammonio)-  
 $\beta$ -D-glucopyranosyl-(1 $\rightarrow$ 4)-O- $\beta$ -D-glucopyranuronosyl-  
 (1 $\rightarrow$ 3)-6-O-[[[(5-amino-2-hydroxybenzoyl)oxy]methyl]-2-deoxy-2-  
 (trimethylammonio)- (9CI) (CA INDEX NAME)

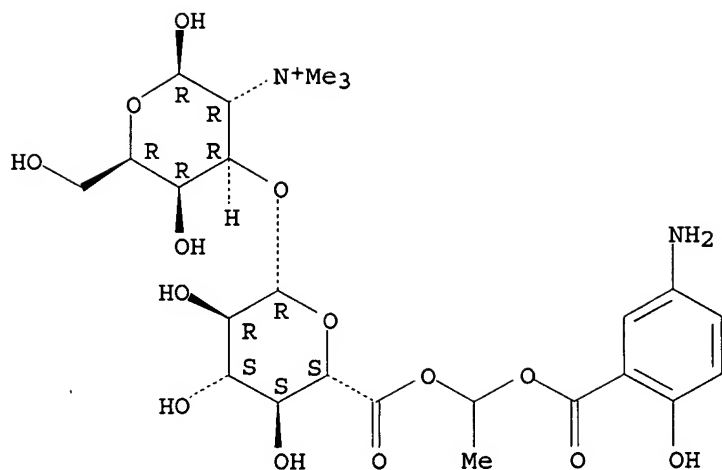
Absolute stereochemistry.



RN 722500-36-9 CAPLUS

CN  $\beta$ -D-Galactopyranose, 3-O-[6-[1-[(5-amino-2-hydroxybenzoyl)oxy]ethyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

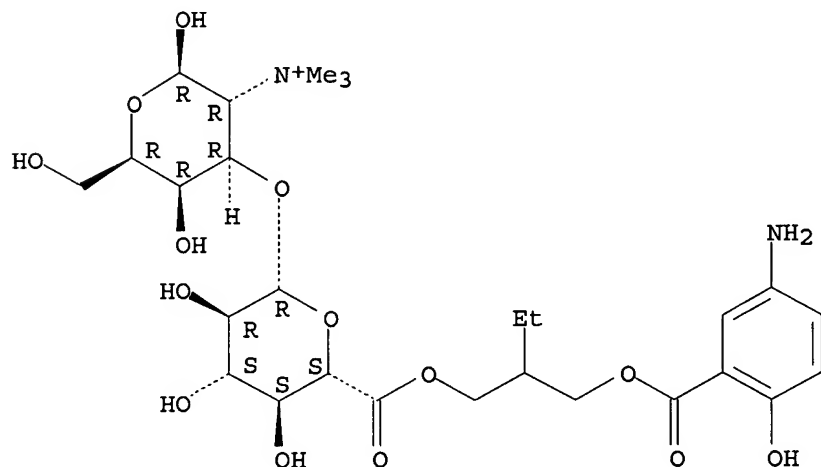
Absolute stereochemistry.



RN 722500-39-2 CAPLUS

CN  $\beta$ -D-Galactopyranose, 3-O-[6-[2-[[[(5-amino-2-hydroxybenzoyl)oxy)methyl]butyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



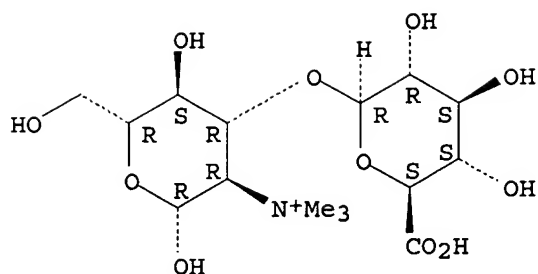
IT 722500-43-8P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of aminodeoxy oligosaccharide as anti-inflammatory agents and their bio-adhesive pharmaceutical compns.)

RN 722500-43-8 CAPLUS

CN  $\beta$ -D-Glucopyranose, 2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 664342-92-1P

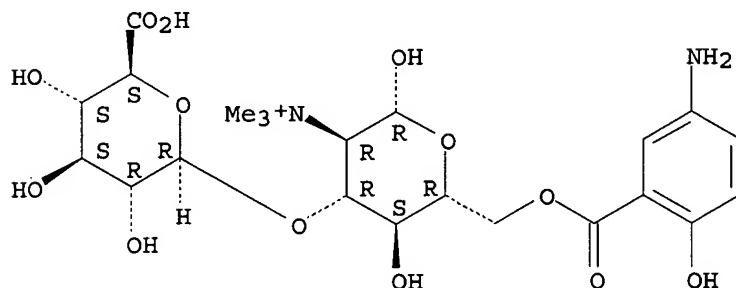
RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminodeoxy oligosaccharide as anti-inflammatory agents and their bio-adhesive pharmaceutical compns.)

RN 664342-92-1 CAPLUS

CN  $\beta$ -D-Glucopyranose, 2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-2-(trimethylammonio)-, 6-(5-amino-2-hydroxybenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L22 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:176557 CAPLUS

DOCUMENT NUMBER: 140:223290

TITLE: Bioadhesive anti-inflammatory aminosalicylate conjugates

INVENTOR(S): Barbeau, Donald L.

PATENT ASSIGNEE(S): USA

SOURCE: U.S., 40 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6699848	B1	20040302	US 2003-348851	20030122
US 2004142880	A1	20040722	US 2004-760970	20040120
CA 2513304	AA	20040805	CA 2004-2513304	20040121
WO 2004064754	A2	20040805	WO 2004-US1536	20040121
WO 2004064754	A3	20050317		
WO 2004064754	C1	20050825		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI				
EP 1585530	A2	20051019	EP 2004-704063	20040121
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
 PRIORITY APPLN. INFO.: US 2003-348851 A2 20030122  
 US 2004-604322 A 20040120  
 US 2004-760970 A 20040120  
 WO 2004-US1536 W 20040121

OTHER SOURCE(S): MARPAT 140:223290

AB Bioadhesive formulations for oral controlled delivery of aminosalicylate (e.g., mesalamine) conjugates with a mono-, di-, or oligosaccharide are described for treatment of inflammatory bowel disease, i.e., Crohn's disease and ulcerative colitis.

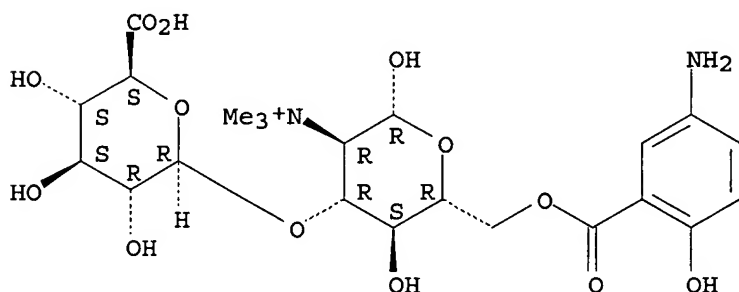
IT 664342-92-1 664342-93-2 664342-94-3

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (aminosalicylate conjugates with saccharide for controlled bioadhesive oral delivery in treatment of inflammatory bowel disease)

RN 664342-92-1 CAPLUS

CN  $\beta$ -D-Glucopyranose, 2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-2-(trimethylammonio)-, 6-(5-amino-2-hydroxybenzoate) (9CI) (CA INDEX NAME)

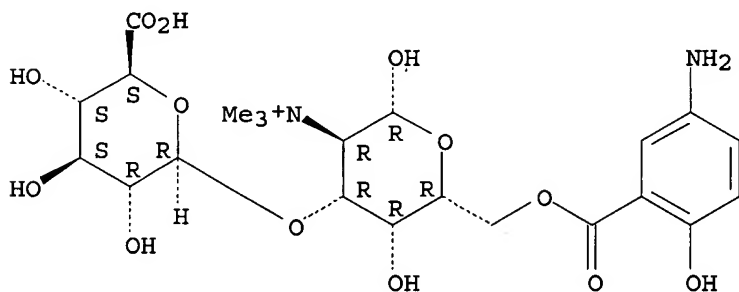
Absolute stereochemistry.



RN 664342-93-2 CAPLUS

CN  $\beta$ -D-Galactopyranose, 2-deoxy-3-O- $\beta$ -D-glucopyranuronosyl-2-(trimethylammonio)-, 6-(5-amino-2-hydroxybenzoate) (9CI) (CA INDEX NAME)

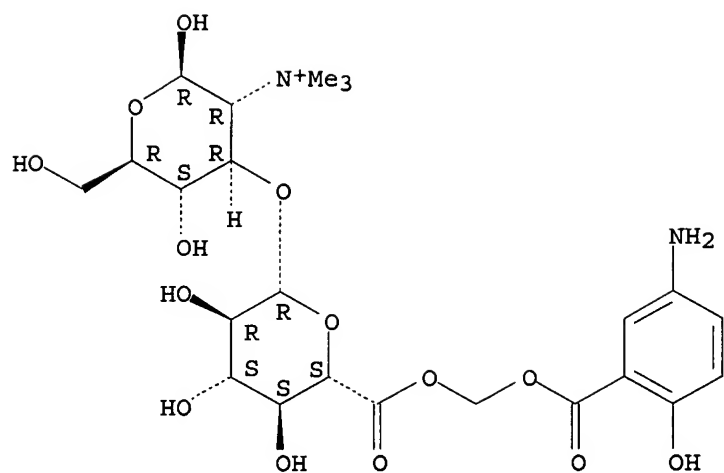
Absolute stereochemistry.



RN 664342-94-3 CAPLUS

CN  $\beta$ -D-Glucopyranose, 3-O-[6-[[5-amino-2-hydroxybenzoyl]oxy]methyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

1

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ACCESSION NUMBER: 2004:589230 CAPLUS

DOCUMENT NUMBER: 141:123864

TITLE: Preparation of aminodeoxy oligosaccharide as anti-inflammatory agents and their bio-adhesive pharmaceutical compositions

INVENTOR(S): Barbeau, Donald L.

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 42 pp., Cont.-in-part of U.S. Ser. No. 348,851.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

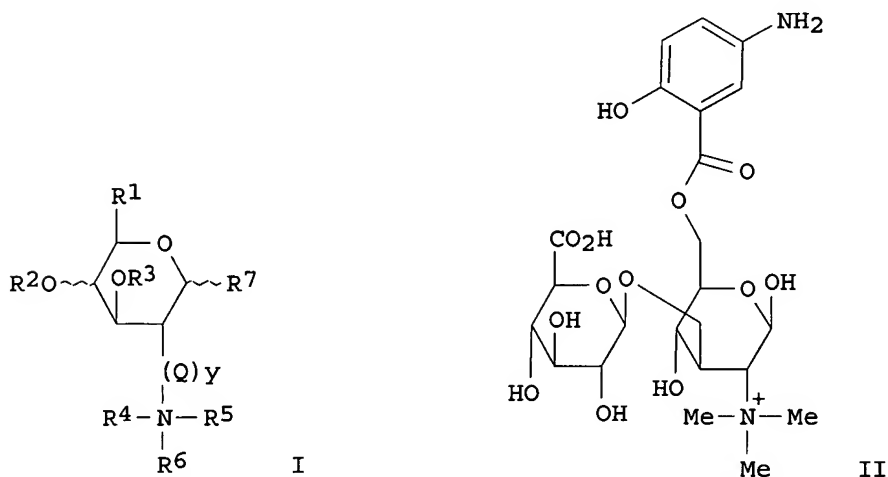
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004142880	A1	20040722	US 2004-760970	20040120
US 6699848	B1	20040302	US 2003-348851	20030122
CA 2513304	AA	20040805	CA 2004-2513304	20040121
PRIORITY APPLN. INFO.:			US 2003-348851	A2 20030122
			US 2004-760970	A 20040120
			WO 2004-US1536	W 20040121

OTHER SOURCE(S): MARPAT 141:123864

GI



AB Aminodeoxy sugars I, wherein Q is a lower alkylene, R<sup>1</sup> is CH<sub>2</sub>-O-(linker)n-R, CO-O-(linker)n-R, CO-NH-(linker)n-R; n is 0, 1; yr is 0, 1; R is H, pharmacol. active drug residue; R<sup>2</sup> is H, monosaccharide residue, oligosaccharide residue; R<sup>3</sup> is H, monosaccharide residue, oligosaccharide residue, CH(CH<sub>2</sub>)C(O)OCH<sub>2</sub>OR<sub>8</sub>; a monomeric glycoside or an oligomeric glycoside; R<sup>4</sup>-R<sup>6</sup> are independently hydrogen, alkyl, aryl, aralkyl, and cycloalkyl or together form a nitrogen-containing ring, and R<sup>7</sup> is hydroxyl or hydroxyalkyl; R<sub>8</sub> a pharmacol. active drug residue. The chronic inflammation in Crohn's disease involves any level of the gastrointestinal tract, and leads to progressive damage in the mucosa, submucosa, the deeper longitudinal muscle layers serosa and regional lymph nodes. Crohn's disease involvement of the mucosa includes confluent linear ulceration patchy, and sharply demarcated granulomas. Thus,

disaccharide uronate II was prepared and tested as anti-inflammatory agent. The invention further relates to a method of controlling the delivery of anti-inflammatory compds., particularly mesalamine (5-amino salicylic acid, 5-ASA), 4-amino salicylic acid (4-ASA), and 3-amino salicylic acid (3-ASA) to the entire gastrointestinal (GI) tract in patients suffering from inflammatory bowel disease. The compns. of the present invention can target a site throughout the length of the gastrointestinal intestinal tract to consistently deliver the medicine where it will be clin. most effective. The compds. of the present invention are characterized by low octanol:water coeffs. and mol. wts. greater than about 300 g/mol. The prodrugs of the present invention are further characterized by their functional properties, including but not limited to bio-adhesion and controlled hydrolysis of the active anti-inflammatory compds.

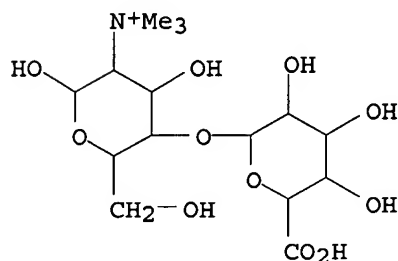
IT 722500-08-5P 722500-24-5P 722500-25-6P

RL: IMF (Industrial manufacture); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of aminodeoxy oligosaccharide as anti-inflammatory agents and their bio-adhesive pharmaceutical compns.)

RN 722500-08-5 CAPLUS

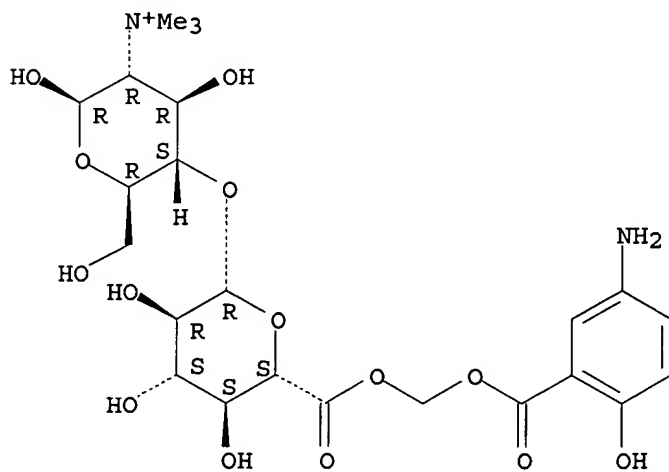
CN Hexopyranose, 2-deoxy-4-O-hexopyranuronosyl-2-(trimethylammonio)- (9CI)  
(CA INDEX NAME)



RN 722500-24-5 CAPLUS

CN  $\beta$ -D-Glucopyranose, 4-O-[6-[[[(5-amino-2-hydroxybenzoyl)oxy]methyl]- $\beta$ -D-glucopyranuronosyl]-2-deoxy-2-(trimethylammonio)- (9CI) (CA INDEX NAME)

Absolute stereochemistry:



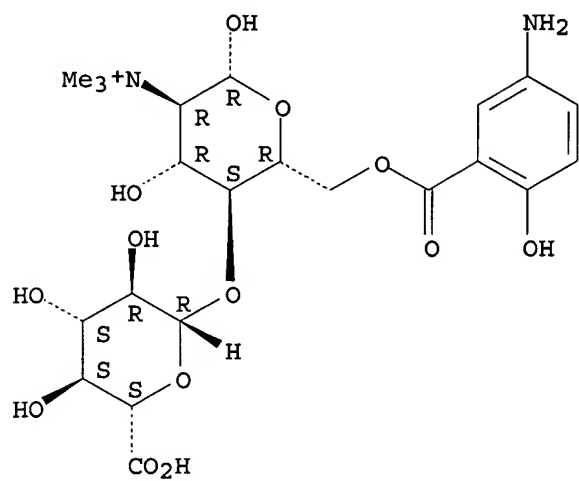
RN 722500-25-6 CAPLUS

CN  $\beta$ -D-Glucopyranose, 2-deoxy-4-O- $\beta$ -D-glucopyranuronosyl-2-



(trimethylammonio)-, 6-(5-amino-2-hydroxybenzoate) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



=> d his

(FILE 'HOME' ENTERED AT 16:50:55 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 16:51:05 ON 13 APR 2006

L1           STRUCTURE UPLOADED  
L2           0 S L1 SSS SAM  
L3           4 S L1 SSS FULL  
L4           STRUCTURE UPLOADED  
L5           1 S L4 SSS SAM  
L6           13 S L4 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 16:57:31 ON 13 APR 2006

L7           4 S L3  
L8           5 S L6

FILE 'REGISTRY' ENTERED AT 17:08:14 ON 13 APR 2006

L9           STRUCTURE UPLOADED  
L10          0 S L9 SSS SAM  
L11          4 S L9 SSS FULL  
L12          STRUCTURE UPLOADED  
L13          1 S L12 SSS SAM  
L14          13 S L12 SSS FULL  
L15          STRUCTURE UPLOADED  
L16          1 S L15 SSS SAM  
L17          15 S L15 SSS FULL  
L18          STRUCTURE UPLOADED  
L19          0 S L18 SSS SAM  
L20          3 S L18 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:24:49 ON 13 APR 2006

L21          2 S L17

FILE 'REGISTRY' ENTERED AT 17:25:31 ON 13 APR 2006

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:25:35 ON 13 APR 2006

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:26:37 ON 13 APR 2006

L22          2 S L17  
L23          1 S L20

=> d his

(FILE 'HOME' ENTERED AT 16:50:55 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 16:51:05 ON 13 APR 2006

L1           STRUCTURE UPLOADED  
L2           0 S L1 SSS SAM  
L3           4 S L1 SSS FULL  
L4           STRUCTURE UPLOADED  
L5           1 S L4 SSS SAM  
L6           13 S L4 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 16:57:31 ON 13 APR 2006

L7           4 S L3  
L8           5 S L6

FILE 'REGISTRY' ENTERED AT 17:08:14 ON 13 APR 2006

L9           STRUCTURE UPLOADED  
L10          0 S L9 SSS SAM  
L11          4 S L9 SSS FULL  
L12          STRUCTURE UPLOADED  
L13          1 S L12 SSS SAM  
L14          13 S L12 SSS FULL  
L15          STRUCTURE UPLOADED  
L16          1 S L15 SSS SAM  
L17          15 S L15 SSS FULL  
L18          STRUCTURE UPLOADED  
L19          0 S L18 SSS SAM  
L20          3 S L18 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:24:49 ON 13 APR 2006

L21          2 S L17

FILE 'REGISTRY' ENTERED AT 17:25:31 ON 13 APR 2006

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:25:35 ON 13 APR 2006

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:26:37 ON 13 APR 2006

L22          2 S L17  
L23          1 S L20

=> d his

(FILE 'HOME' ENTERED AT 16:50:55 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 16:51:05 ON 13 APR 2006

L1           STRUCTURE UPLOADED  
L2           0 S L1 SSS SAM  
L3           4 S L1 SSS FULL  
L4           STRUCTURE UPLOADED  
L5           1 S L4 SSS SAM  
L6           13 S L4 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 16:57:31 ON 13 APR 2006

L7           4 S L3  
L8           5 S L6

FILE 'REGISTRY' ENTERED AT 17:08:14 ON 13 APR 2006

L9           STRUCTURE UPLOADED  
L10          0 S L9 SSS SAM  
L11          4 S L9 SSS FULL  
L12          STRUCTURE UPLOADED  
L13          1 S L12 SSS SAM  
L14          13 S L12 SSS FULL  
L15          STRUCTURE UPLOADED  
L16          1 S L15 SSS SAM  
L17          15 S L15 SSS FULL  
L18          STRUCTURE UPLOADED  
L19          0 S L18 SSS SAM  
L20          3 S L18 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:24:49 ON 13 APR 2006

L21          2 S L17

FILE 'REGISTRY' ENTERED AT 17:25:31 ON 13 APR 2006

FILE 'CAPLUS, MEDLINE' ENTERED AT 17:25:35 ON 13 APR 2006

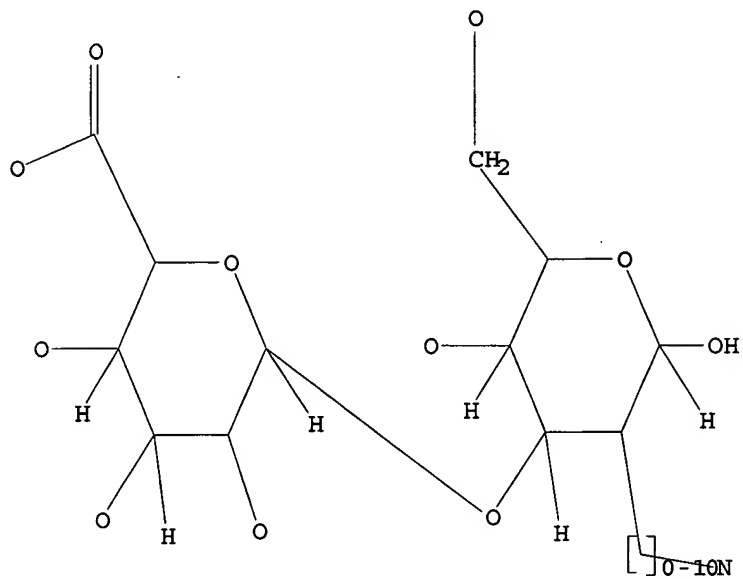
FILE 'CAPLUS, MEDLINE' ENTERED AT 17:26:37 ON 13 APR 2006

L22          2 S L17  
L23          1 S L20

=>  
Uploading C:\Program Files\Stnexp\Queries\10760970-i.str

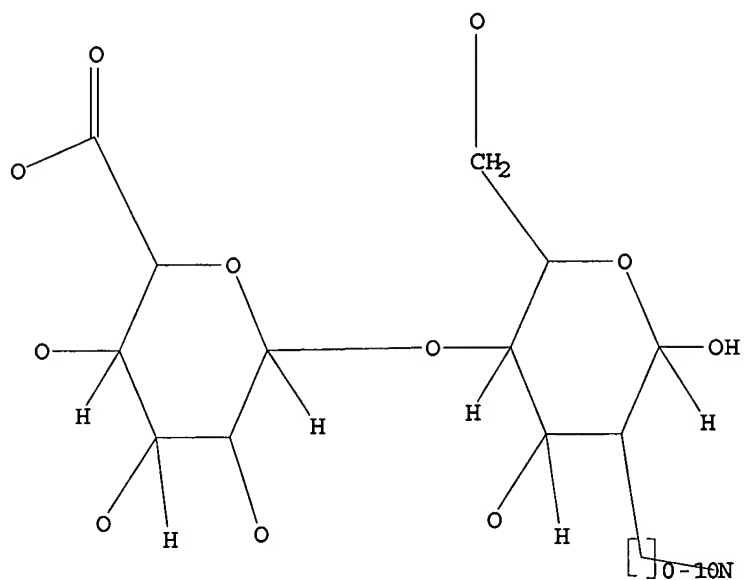
L1        STRUCTURE UPLOADED

=> d L1  
L1 HAS NO ANSWERS  
L1        STR



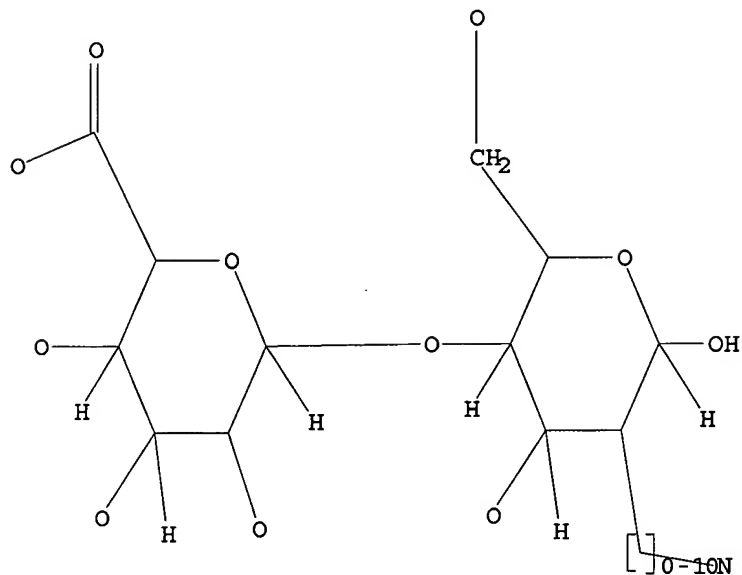
Structure attributes must be viewed using STN Express query preparation.

=> d 14  
L4 HAS NO ANSWERS  
L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> d l4  
 L4 HAS NO ANSWERS  
 L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L4 sss sam  
 SAMPLE SEARCH INITIATED 17:36:50 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 1269 TO ITERATE

100.0% PROCESSED 1269 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 23243 TO 27517  
 PROJECTED ANSWERS: 0 TO 0

L5 0 SEA SSS SAM L4

=> s L4 sss full  
 FULL SEARCH INITIATED 17:36:55 FILE 'REGISTRY'  
 SCREENING  
 FULL SCREEN SEARCH COMPLETED - 25560 TO ITERATE

100.0% PROCESSED 25560 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

L6 0 SEA SSS FUL L4

=> d his

(FILE 'HOME' ENTERED AT 17:33:52 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 17:34:04 ON 13 APR 2006

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	1 S L1 SSS FULL
L4	STRUCTURE UPLOADED
L5	0 S L4 SSS SAM
L6	0 S L4 SSS FULL



=> d his

(FILE 'HOME' ENTERED AT 17:33:52 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 17:34:04 ON 13 APR 2006

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	1 S L1 SSS FULL
L4	STRUCTURE UPLOADED
L5	0 S L4 SSS SAM
L6	0 S L4 SSS FULL

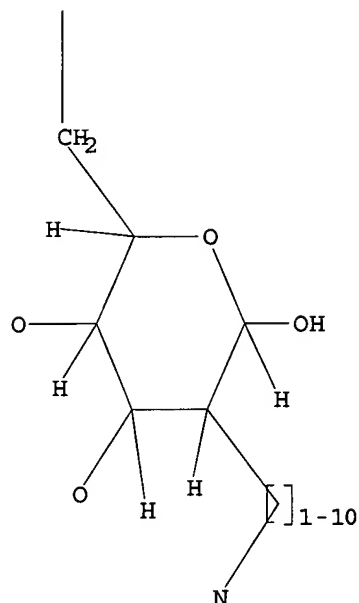
=> d his

(FILE 'HOME' ENTERED AT 17:33:52 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 17:34:04 ON 13 APR 2006

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	1 S L1 SSS FULL
L4	STRUCTURE UPLOADED
L5	0 S L4 SSS SAM
L6	0 S L4 SSS FULL

```
=> d L1
L1 HAS NO ANSWERS
L1 STR
```



Structure attributes must be viewed using STN Express query preparation.

```
=> s L1 sss sam
SAMPLE SEARCH INITIATED 15:06:00 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED      15 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   68 TO      532
PROJECTED ANSWERS:      0 TO      0
```

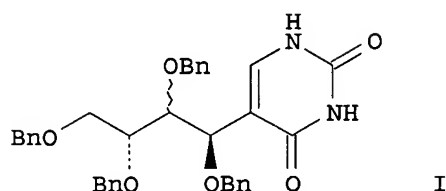
```
L2      0 SEA SSS SAM L1
```

```
=> s L1 sss full
FULL SEARCH INITIATED 15:06:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 162 TO ITERATE
```

```
100.0% PROCESSED      162 ITERATIONS      9 ANSWERS
SEARCH TIME: 00.00.01
```

```
L3      9 SEA SSS FUL L1
```

L10 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1996:334944 CAPLUS  
 DOCUMENT NUMBER: 125:87084  
 TITLE: Synthesis of 5-tetrahydroxybutyl-uracil derivatives  
 from benzylated D-glucal and D-galactal  
 AUTHOR(S): Mostowicz, D.; Chmielewski, M.  
 CORPORATE SOURCE: Inst. Org. Chem., Polish Acad. Sci., Warsaw, 01-224,  
 Pol.  
 SOURCE: Carbohydrate Letters (1994), 1(2), 95-98  
 CODEN: CLETEC; ISSN: 1073-5070  
 PUBLISHER: Harwood  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Two diastereomeric acyclic C-nucleosides I were prepared from D-glucal and D-galactal. Synthesis involved [2+2] cycloaddn. of glycal to trichloroacetyl isocyanate or chlorosulfonyl isocyanate, carbamoylation of the  $\beta$ -lactam nitrogen atom, opening of the four-membered ring with methanol and intramol. cyclocondensation of glycosyl urea to the resp. uracil.

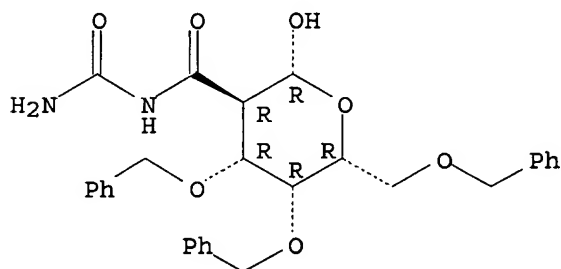
IT 178681-27-1P 178681-31-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of tetrahydroxybutyluracils from benzylated glucal and galactal)

RN 178681-27-1 CAPLUS

CN  $\beta$ -D-Galactopyranose, 2-[[[(aminocarbonyl)amino]carbonyl]-2-deoxy-3,4,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

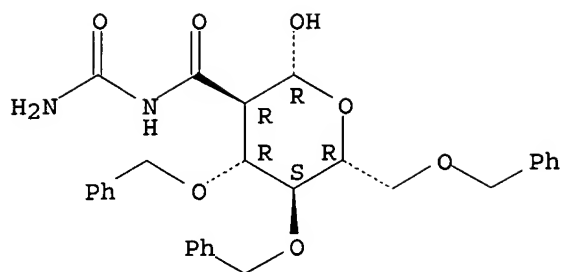
Absolute stereochemistry.



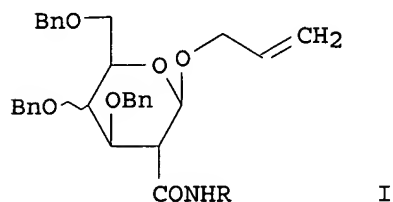
RN 178681-31-7 CAPLUS

CN  $\beta$ -D-Glucopyranose, 2-[[[(aminocarbonyl)amino]carbonyl]-2-deoxy-3,4,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

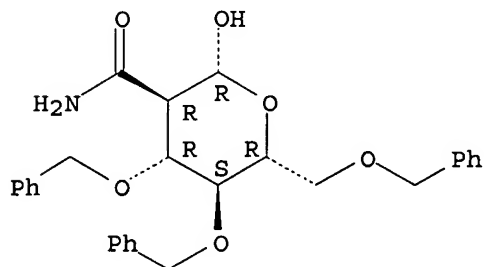


L10 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN  
 ACCESSION NUMBER: 1995:21634 CAPLUS  
 DOCUMENT NUMBER: 122:161132  
 TITLE: Unexpected course of deprotection of allyl ethers  
 AUTHOR(S): Mostowicz, D.; Chmielewski, M.  
 CORPORATE SOURCE: Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, 01-224, Pol.  
 SOURCE: Polish Journal of Chemistry (1993), 67(7), 1235-41  
 CODEN: PJCHDQ; ISSN: 0137-5083  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 122:161132  
 GI



AB Various allyl 2-carbamoyl-2-deoxyglycopyranosides and their N-carbamoyl derivs., e.g. I (R = H, CONH2), were synthesized. Deprotection of the allyl ether function with palladium chloride-sodium acetate-acetic acid mixture led to 2'-ketopropyl glycosides. Deallylation was achieved by applying Wilkinson's catalyst.  
 IT 161045-00-7P 161045-01-8P 161045-05-2P  
 161045-06-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (deallylation of allyl carbamoyldeoxyglycopyranosides in presence of Wilkinson's catalyst)  
 RN 161045-00-7 CAPLUS  
 CN  $\beta$ -D-Glucopyranose, 2-(aminocarbonyl)-2-deoxy-3,4,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

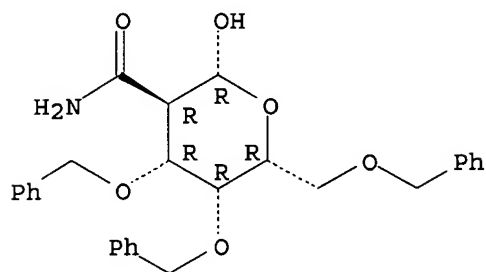
Absolute stereochemistry.



RN 161045-01-8 CAPLUS

CN  $\beta$ -D-Galactopyranose, 2-(aminocarbonyl)-2-deoxy-3,4,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

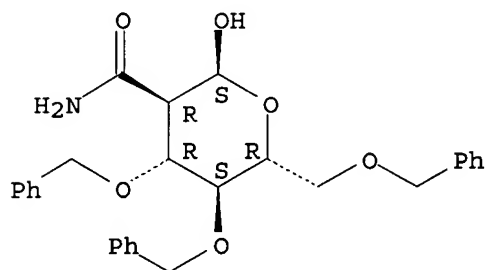
Absolute stereochemistry.



RN 161045-05-2 CAPLUS

CN  $\alpha$ -D-Glucopyranose, 2-(aminocarbonyl)-2-deoxy-3,4,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

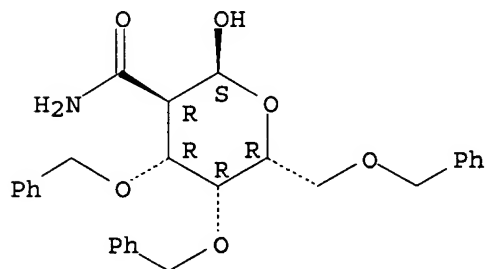
Absolute stereochemistry.



RN 161045-06-3 CAPLUS

CN  $\alpha$ -D-Galactopyranose, 2-(aminocarbonyl)-2-deoxy-3,4,6-tris-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L10 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1993:169493 CAPLUS

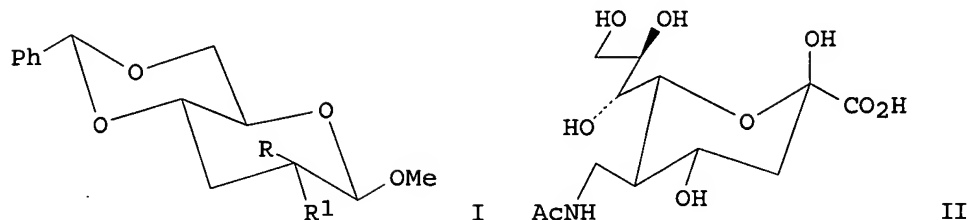
DOCUMENT NUMBER: 118:169493

TITLE: Synthesis of the C-5 homolog of N-acetylneuraminic acid by enzymic chain elongation of 2-C-acetamidomethyl-2-deoxy-D-mannose

AUTHOR(S): Koppert, Klaus; Brossmer, Reinhard

CORPORATE SOURCE: Inst. Biochem. II, Univ. Heidelberg, Heidelberg, 6900, Germany

SOURCE: Tetrahedron Letters (1992), 33(52), 8031-4  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 118:169493  
 GI



AB Condensation of hexopyranosid-2-ulose I (RR1 = O) with MeNO<sub>2</sub> and acetylation gave I (R = OAc, R1 = CH<sub>2</sub>NO<sub>2</sub>; R = CH<sub>2</sub>NO<sub>2</sub>, R1 = OAc). Subsequent treatment with NaBH<sub>4</sub> gave I (R = CH<sub>2</sub>NO<sub>2</sub>, R1 = H) stereoselectively. Reduction, acetylation, deblocking, and acid hydrolysis gave the C-2 branched N-acetylmannosamine which was enzymically converted to the first known C-5 branched homolog II of acetylneuraminic acid.

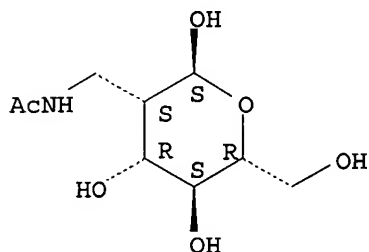
IT 146668-93-1P 146668-94-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation and enzymic chain elongation of, with pyruvate)

RN 146668-93-1 CAPLUS

CN α-D-Mannopyranose, 2-[(acetylamino)methyl]-2-deoxy- (9CI) (CA INDEX NAME)

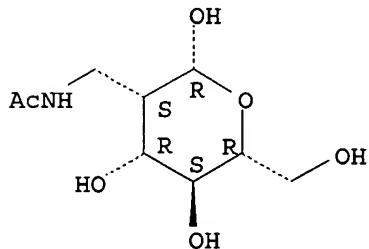
Absolute stereochemistry.



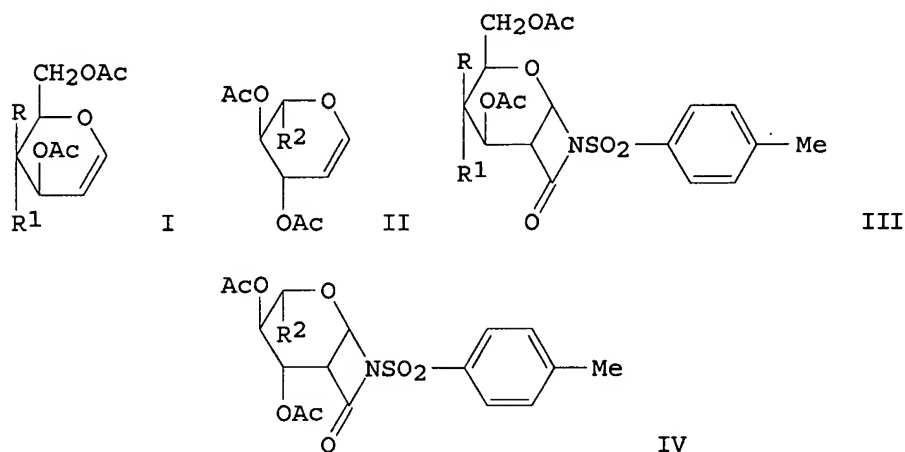
RN 146668-94-2 CAPLUS

CN β-D-Mannopyranose, 2-[(acetylamino)methyl]-2-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

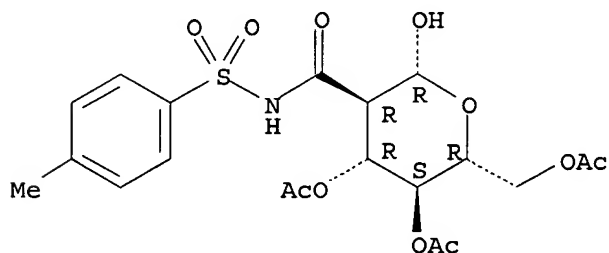


ACCESSION NUMBER: 1985:113769 CAPLUS  
 DOCUMENT NUMBER: 102:113769  
 TITLE: The synthesis of optically pure  $\beta$ -lactams derived from sugars. High-pressure [2 + 2] cycloaddition of toluene-4-sulfonyl isocyanate to glycals  
 AUTHOR(S): Chmielewski, M.; Kaluza, Z.; Belzecki, C.; Salanski, P.; Jurczak, J.  
 CORPORATE SOURCE: Inst. Org. Chem., Polish Acad. Sci., Warsaw, 01-224, Pol.  
 SOURCE: Tetrahedron Letters (1984), 25(42), 4797-800  
 CODEN: TELEAY; ISSN: 0040-4039  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



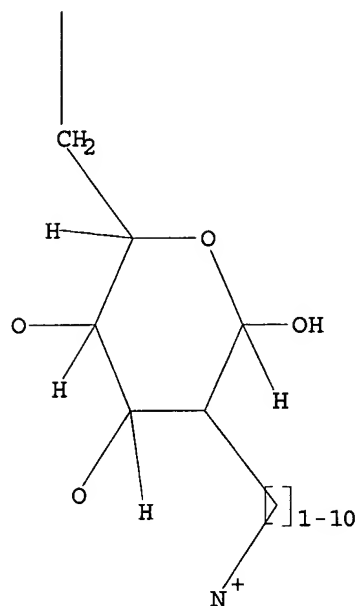
AB [2+2] Cycloaddn. of 4-MeC<sub>6</sub>H<sub>4</sub>SO<sub>2</sub>NCO to glycals at room I (R = OAc, [R<sub>1</sub> = H; R = H, R<sub>1</sub> = OAc) and II (R<sub>2</sub> = H, Me) at room temperature under 10 kbar pressure gave  $\beta$ -lactams III and IV, resp., in good yields. The reaction proceeds regio- and stereospecifically to afford the 4-membered ring in position trans to the acetoxy group at C-3 of the glycal moiety.  
 IT 95068-78-3P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
     (preparation of)  
 RN 95068-78-3 CAPLUS  
 CN  $\beta$ -D-Glucopyranose, 2-deoxy-2-[[[(4-methylphenyl) sulfonyl] amino] carbon  
     yl]-, 3,4,6-triacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.





```
=> d L4
L4 HAS NO ANSWERS
L4 STR
```



Structure attributes must be viewed using STN Express query preparation.

```
=> s L4 sss sam
SAMPLE SEARCH INITIATED 15:12:32 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE
```

```
100.0% PROCESSED      15 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.01
```

```
FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:   68 TO    532
PROJECTED ANSWERS:      0 TO     0
```

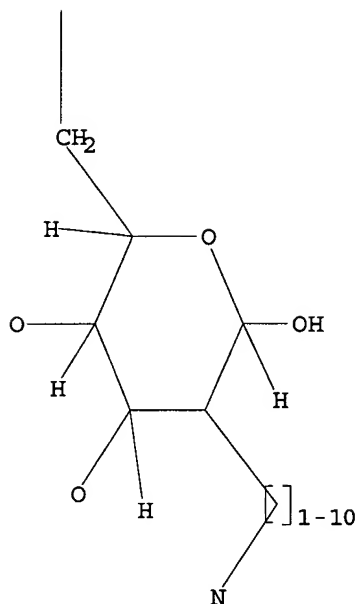
```
L5      0 SEA SSS SAM L4
```

```
=> s L4 sss full
FULL SEARCH INITIATED 15:12:38 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 162 TO ITERATE
```

```
100.0% PROCESSED      162 ITERATIONS      0 ANSWERS
SEARCH TIME: 00.00.01
```

```
L6      0 SEA SSS FUL L4
```

=> d 17  
 L7 HAS NO ANSWERS  
 L7 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L7 sss sam  
 SAMPLE SEARCH INITIATED 15:15:04 FILE 'REGISTRY'  
 SAMPLE SCREEN SEARCH COMPLETED - 15 TO ITERATE

100.0% PROCESSED 15 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
 BATCH \*\*COMPLETE\*\*  
 PROJECTED ITERATIONS: 68 TO 532  
 PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

=> s L7 sss full  
 FULL SEARCH INITIATED 15:15:10 FILE 'REGISTRY'  
 FULL SCREEN SEARCH COMPLETED - 162 TO ITERATE

100.0% PROCESSED 162 ITERATIONS 0 ANSWERS  
 SEARCH TIME: 00.00.01

L9 0 SEA SSS FUL L7

=> d his

(FILE 'HOME' ENTERED AT 15:05:27 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 15:05:37 ON 13 APR 2006

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	9 S L1 SSS FULL
L4	STRUCTURE UPLOADED
L5	0 S L4 SSS SAM
L6	0 S L4 SSS FULL
L7	STRUCTURE UPLOADED
L8	0 S L7 SSS SAM
L9	0 S L7 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 15:20:04 ON 13 APR 2006

L10	4 S L3
-----	--------

=> d his

(FILE 'HOME' ENTERED AT 15:05:27 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 15:05:37 ON 13 APR 2006

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	9 S L1 SSS FULL
L4	STRUCTURE UPLOADED
L5	0 S L4 SSS SAM
L6	0 S L4 SSS FULL
L7	STRUCTURE UPLOADED
L8	0 S L7 SSS SAM
L9	0 S L7 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 15:20:04 ON 13 APR 2006

L10	4 S L3
-----	--------

=> d his

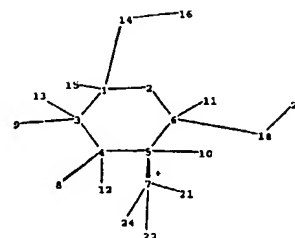
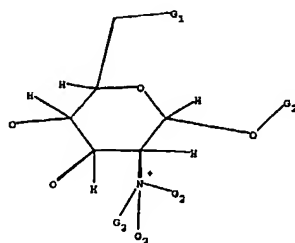
(FILE 'HOME' ENTERED AT 15:05:27 ON 13 APR 2006)

FILE 'REGISTRY' ENTERED AT 15:05:37 ON 13 APR 2006

L1	STRUCTURE UPLOADED
L2	0 S L1 SSS SAM
L3	9 S L1 SSS FULL
L4	STRUCTURE UPLOADED
L5	0 S L4 SSS SAM
L6	0 S L4 SSS FULL
L7	STRUCTURE UPLOADED
L8	0 S L7 SSS SAM
L9	0 S L7 SSS FULL

FILE 'CAPLUS, MEDLINE' ENTERED AT 15:20:04 ON 13 APR 2006

L10	4 S L3
-----	--------



chain nodes :

7 8 9 10 11 12 13 14 15 16 18 20 21 22 24

ring nodes :

1 2 3 4 5 6

chain bonds :

1-15 1-14 3-9 3-13 4-8 4-12 5-7 5-10 6-11 6-18 7-21 7-22 7-24 14-16 18-20

ring bonds :

1-3 1-2 2-6 3-4 4-5 5-6

exact/norm bonds :

1-3 1-2 2-6 3-4 3-9 4-5 4-8 5-6 5-7 6-18 7-21 7-22 7-24 14-16 18-20

exact bonds :

1-15 1-14 3-13 4-12 5-10 6-11

G1:O,NH

G2:C,H

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 18:CLASS 20:CLASS 21:CLASS  
22:CLASS 24:CLASS

Stereo Bonds:

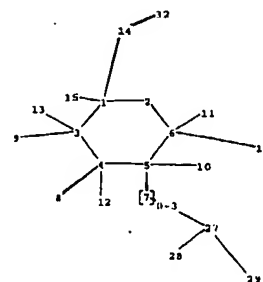
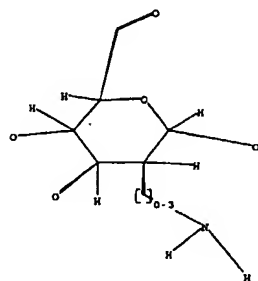
7-5 (Single Hash).  
8-4 (Single wedge).  
14-1 (Single wedge).

Stereo Chiral Centers:

1 (Parity=Even)  
4 (Parity=Even)  
5 (Parity=Odd)

Stereo RSS Sets:

Type=Relative (Default). 3 Nodes= 1 4 5



chain nodes :

7 8 9 10 11 12 13 14 15 16 27 28 29 32

ring nodes :

1 2 3 4 5 6

chain bonds :

1-15 1-14 3-9 3-13 4-8 4-12 5-7 5-10 6-11 6-16 7-27 14-32 27-28 27-29

ring bonds :

1-3 1-2 2-6 3-4 4-5 5-6

exact/norm bonds :

1-3 1-2 2-6 3-4 3-9 4-5 4-8 5-6 6-16 7-27 14-32

exact bonds :

1-15 1-14 3-13 4-12 5-7 5-10 6-11 27-28 27-29

G2:H,CH2,CH

G3:C,H

G4:H,O

Match level :

1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS  
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 27:CLASS 28:CLASS 29:CLASS  
32:CLASS

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Stereo chiral Centers:

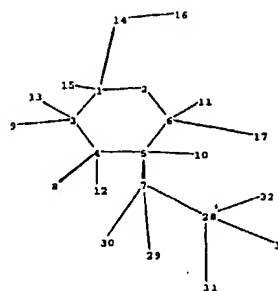
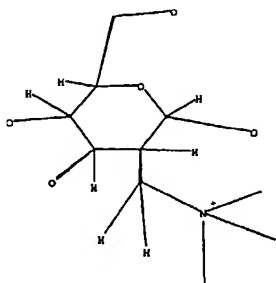
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chain nodes :

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ring nodes :

1 2 3 4 5 6

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G3:C,H

G4:H,O

Match level :

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11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 28:CLASS 29:CLASS  
30:CLASS 31:CLASS 32:CLASS 33:CLASS

Stereo Bonds:

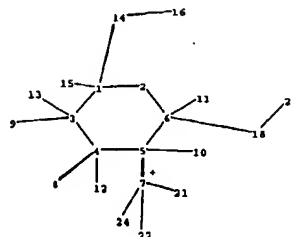
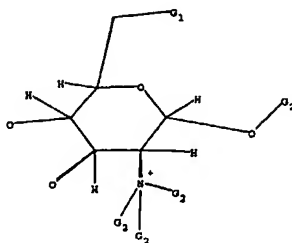
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